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Dilution attenuation factors in susceptibility assessments: A GIS based method

by

Gil Strassberg, M.S.E.

Graduate Research Assistant

and

David R. Maidment, Ph.D.

Lynn E. Katz, ph.D.

Principle Investigators

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Bureau of Engineering Research • The University of Texas at Austin

J.J. Pickle Research Campus • Austin, TX 78712-4497

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Gil Strassberg

Report

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DEDICATION

To my family

ACKNOWLEDGEMENTS

I would like to thank those that made this study and report possible. First to my advisors Dr. Maidment and Dr. Katz, I am grateful for your support and guidance throughout the project. I would also like to thank the USGS and TCEQ SWAP teams for their professional assistance and financial support. Special thanks to Randy Ulery, Brian Reece and Richard Kiesling, from USGS, and John Meyer and Greg Rogers, from TCEQ, for your personal assistance. Lastly, I would like to thank the CRWR research group for their friendship, assistance and team work. You all made this an exciting and educating experience.

ABSTRACT

Dilution attenuation factors in susceptibility assessments: A GIS based method

Gil Strassberg, M.S.E.

The University of Texas at Austin, 2003

Supervisor: David R. Maidment

The 1996 Amendments to the Safe Drinking Water Act require each state to prepare a source water assessment for all public water supplies, emphasizing the importance of protecting water sources. States are required to determine the drinking water source and the origin of contaminants for each public water supply. These assessments determine the susceptibility of individual water sources to contamination from various sources of contamination.

The Texas Source Water Assessment Program is a joint effort of the U.S. Geological Survey (USGS) and the Texas Commission on Environmental Quality (TCEQ). Its objective is to construct a methodology for evaluating the relative susceptibility of Texas' Public Water Supplies (PWS) to contamination. The program is a combination of different source and transport components, that when linked together, yield the final susceptibility assessment.

The work presented focuses on the development of a dilution attenuation factor component that is integrated into the ground water susceptibility

assessment using GIS. This component is based on a Tier 2 screening model presented in the Texas Risk Reduction Program (TRRP). The Tier 2 model is a steady state model that calculates concentration ratios between contaminated soils and groundwater. The model describes the major natural processes taking place in the environment during contaminants migration in groundwater systems. These processes include dilution, sorption, dispersion and degradation Model inputs include soil, aquifer and chemical properties. The output gives a dilution attenuation factor, which is the ratio between the concentration of pollutants in the soil, at the source of contamination, and in the groundwater at the water supply well.

The numerical relationship, between sources of contamination and contaminant concentrations at water supply wells can be used to better estimate the susceptibility of water supplies to contamination.

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1. INTRODUCTION

The 1996 Amendments to the Safe Drinking Water Act require each state to prepare a source water assessment for all public water supplies, emphasizing the importance of protecting water sources. States are required to determine the drinking water source and the origin of contaminants for each public water supply. These assessments determine the susceptibility of individual water sources to contamination. The 1996 amendments resulted in the development of source water assessment programs in each state, supervised by the U.S. EPA.

The Texas Source Water Assessment Program is a joint effort of the US Geological Survey (USGS) and the Texas Commission on Environmental Quality (TCEQ). Its objective is to construct a methodology for evaluating the relative susceptibility of Texas' Public Water Supplies (PWS) to contamination. These assessments may benefit the public by focusing source water protection efforts on highly susceptible water supplies, potentially reduce water supply monitoring costs and support the implementation of best management practices in water supplies. The methodology applied in the Texas Source Water Assessment Program is a combination of different source and transport components, that when linked together, yield the final susceptibility assessment.

The program evaluates surface and groundwater water supplies. This research is focused on the groundwater section of the program, thus only the groundwater section is described. The components of the groundwater assessment include identification of water supplies, delineation of capture zones,

identification of non-point sources of contamination, point sources of contamination and attenuation. The susceptibility assessment begins with the identification of the water supply and the corresponding aquifer. Next, the delineation component defines the contributing area around the well, and point sources of contamination are identified within the contributing zone. Sources are then associated with specific constituents. Finally contaminants dilution and attenuation processes are simulated to determine the concentration of each contaminant at the water supply location.

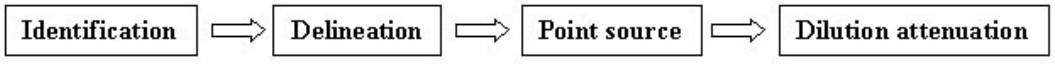

Figure 1 - Groundwater point source susceptibility process

The work presented focuses on the development of a dilution attenuation factor component that can be integrated in the ground water susceptibility assessment. This component is based on a Tier 2 screening model presented in the Texas Risk Reduction Program (TRRP). The Tier 2 model is a steady state model that calculates concentration ratios between contaminated soils and groundwater. The model inputs include soil, aquifer and chemical properties. The output gives a dilution attenuation factor, which is the ratio between the concentration of pollutants in the soil, at the source of contamination, and in the groundwater at the supply well.

Soil screening models are used extensively in risk reduction assessments to help decision making for contaminated soil sites. The screening models consider contaminant migration through the unsaturated zone to the water table

and the mixing of contaminants when they reach the aquifer. This process results in dilution of the contaminant's concentration. Groundwater transport in the saturated zone, to the receptor well, further reduces the concentration through sorption, dispersion and degradation. The dilution attenuation factor combines these processes into one numerical value that relates contaminant concentrations at the source of contamination and the receptor well.

In the Texas source water assessment program over 200 chemicals of concern are assessed for over 850,000 potential sources of contamination and 13,000 water supply wells. Therefore, construction of a computerized method based on Geographic Information Systems (GIS) is ideal for calculating dilution attenuation factors for each source of contamination. The Tier 2 screening model provides a logical method to combine the soil, aquifer and chemical properties into a GIS based method. This method uses GIS capabilities to retrieve source and aquifer properties and compute dilution attenuation factors, which are then used to determine the susceptibility of water supplies to point sources of contamination.

The relationship between the sources identified in each contributing zone and their potential effects on water quality are utilized in determining the susceptibility of wells to contamination. This relationship allows one to not only identify the sources of contamination but to relate them to water quality through a physical model. The results of this model help determine the susceptibility of each well to contamination from potential point sources.

2. TEXAS SOURCE WATER ASSESSMENT PROGRAM

The Texas source water assessment program was mandated to develop a scientifically defensible methodology for assessing the susceptibility of Texas public water supplies to contamination. Susceptibility of a public water supply is defined as *the potential for the public water supply to withdraw water containing a listed contaminant(s), at a concentration that would pose concern* (USGS, 2000). The program is divided into three main subjects: Software and database structure, ground water assessments and surface water assessments.

This study focuses on the groundwater susceptibility section of the program, thus only a detailed description of the groundwater section is provided. Detailed information regarding the surface water component and the software and database structure design are presented in the documentation of the program (USGS, 2000 and USGS, 2002).

The groundwater section of the assessment includes several components combined to assess the susceptibility of public water supply wells. Such components are the identification, delineation of contributing area, point and non point sources, contaminant occurrence, attenuation and susceptibility determination. The complete assessment utilizes the results of all components to yield the final susceptibility assessment. The attenuation component, which is the main subject of this study, is built upon other components in the assessment. Thus a brief description of the identification, delineation and point source components is provided.

2.1 IDENTIFICATION COMPONENT

The first step in a water susceptibility assessment is to identify the source of the water, in the case of groundwater the source refers to the aquifer that the assessed well is deriving its water from. The hydrological and geological characteristics of the aquifer have a major effect on the water quality. Obviously different aquifers will yield varying susceptibilities due to differences in aquifer properties.

Historically, nine major and twenty minor aquifers have been mapped in Texas (Ashworth and Hopkins, 1995). In the source water assessment program these aquifers were subdivided into about 40 aquifer codes for which sufficient aquifer detail is available (USGS, 2002). The aquifers were then assigned an aquifer type, which is used to determine the capture zone. The following aquifer types were used in the program.

1. Unconfined isotropic aquifers
2. Confined isotropic aquifers
3. Alluvial aquifers along major rivers
4. Anisotropic karst aquifers
5. Other aquifers

Aquifer type 5 is used where the well is screened in an aquifer that is not included in the 40 aquifer codes, or when the aquifer type cannot be defined.

The source of the water, aquifer code, is determined for each well in the susceptibility assessment based on screening information. Once the aquifer and aquifer type are identified the contributing zone of the well can be delineated with the delineation component of the assessment.

2.2 DELINEATION OF THE CONTRIBUTING AREA COMPONENT

The contributing area of the well and time of travel are delineated for each public water supply well. A grid based delineation process uses aquifer properties and well draws down to determine the contributing area of the well. Within this area flow paths and velocities can be computed and combined to compute the time of travel to the well.

Different applications are used for varying aquifer types. All methods use a regional potentiometric surface representation of the aquifer and a draw down surface, computed using the Theis equation for unconfined and confined aquifers. The drawdown surface is deducted from the regional potentiometric surface to yield a new surface that describes the actual aquifer potentiometric surface including the influence of well discharges. Once this surface is computed flow paths and velocities can be derived using the gradients in the computed surface and aquifer properties. The following images demonstrate this process, a full description of the delineation processes are detailed in the groundwater section of the program's strategy (Texas Natural Resource Conservation Commission, 1999).

The following example illustrates the computation of the draw down surface and the delineation of the contributing area. In this example two wells create a draw down surface, which is then subtracted from the regional water table to create the actual potentiometric surface. Then the flow direction, and time of travel can be determined and a contributing area can be outlined. Figure 2 shows the summation of the drawdown surfaces (draw down values are given in feet and the grids' cell size is 60 meters).

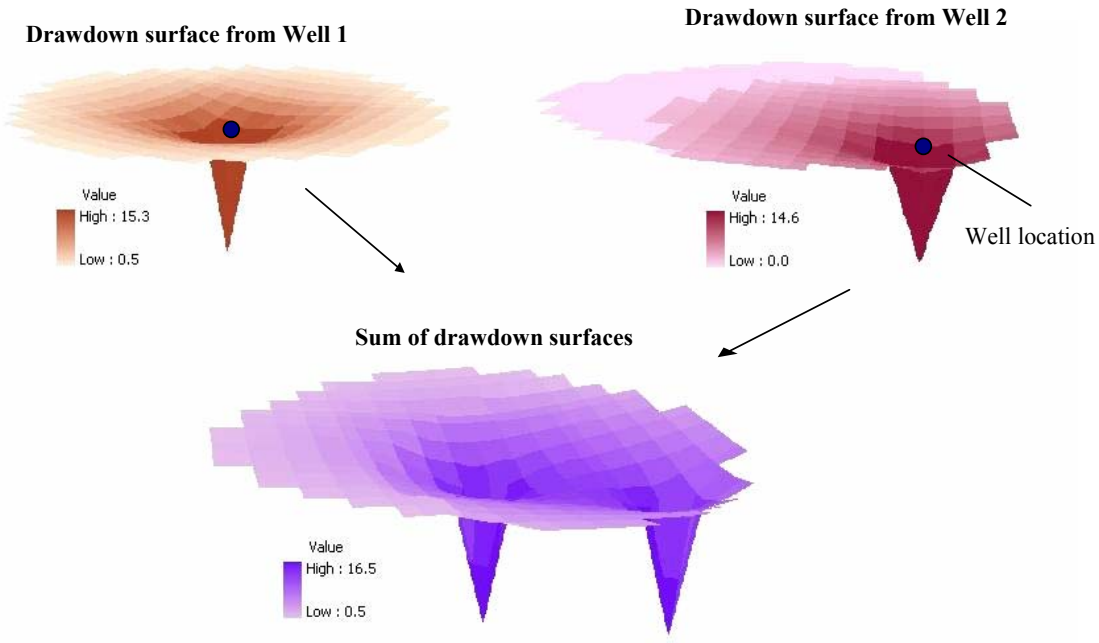

Figure 2 - Creating a drawdown surface from the drawdown of two wells

(cell size of grids 60 meters)

Once the drawdown surface is computed it is deducted from the regional potentiometric surface to create a new surface. This surface describes the actual

potentiometric surface/water table that includes the influence of discharge from multiple wells. From this surface gradients between cells can be computed and flow direction and velocities can be calculated using the gradients, hydraulic conductivity and the aquifer porosity. With the flow direction, flow paths can be determined and a contributing area can be delineated for each well. Using the flow path length and the flow velocity, the time of travel can be computed for each grid cell in the contributing area. Figure 3 shows the delineated area over the drawdown surface and the time of travel, in years, for water to reach the well.

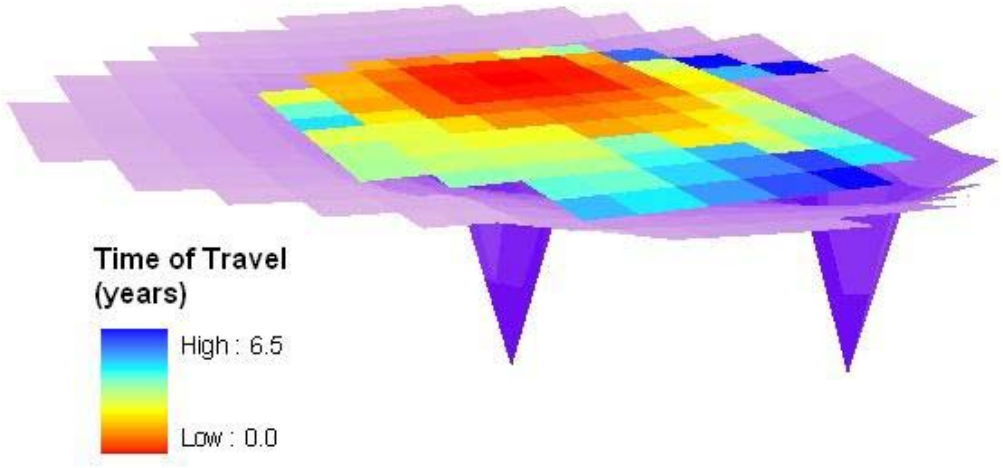

Figure 3 - Contributing area (for well 1) and the delineated time of travel (years)

2.3 POINT SOURCE COMPONENT

In this component, potential point sources of contamination are identified within each delineated contributing area. Point and non point sources may introduce similar contaminants into the environment, but the point sources can be geographically located, assigned coordinates and categorized. In the assessment

each source type is related to a list of contaminants and source properties, such as the extent of the source, are estimated. When a point source of contamination is located in the contributing area of a well, one can use the list of related contaminants and the source properties to assess the impact on water quality at the well. Figure 4 illustrates this process, where coverage of potential sources is intersected with a contributing area. Then the potential sources of contamination and their properties are identified and the results are used as inputs in the dilution attenuation component.

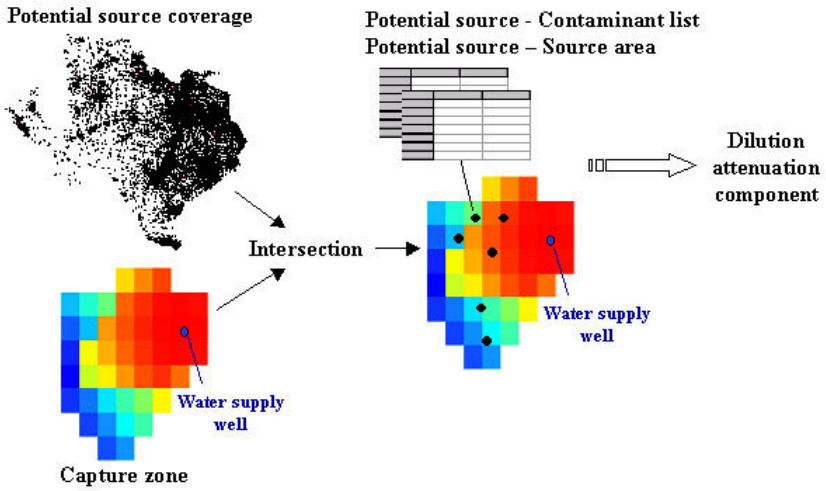

Figure 4 - Identification of point sources of contamination within the capture zone of a well

The processes described in the delineation and point sources component are feasible due to extensive data and application development undertaken in the source water assessment program by the USGS and TCEQ. These processes provide the inputs for the dilution attenuation component described next.

2.4 DILUTION ATTENUATION COMPONENT

Contaminants that are introduced into the ground water environment can undergo chemical, physical and biochemical processes that result in the reduction of contaminant concentrations. A soil-screening model is used to estimate the concentration reduction between the contaminant points of introduction, the potential sources of contamination, and the assessed well.

The soil-screening model used in this component is a Tier 2 model, which is described in the Texas Risk Reduction Program (TRRP, Tier 2 PCL Equations). This is a steady state model that calculates dilution of contaminants leaching from soil layers into the water table and the transport and degradation of the constituents in the aquifer. The model incorporates a two-phased approach for describing the movement of contaminants from the soil, at the source of contamination, to the water supply well.

This component yields a numerical relationship, a dilution attenuation factor, between the source of contamination and the assessed well. This relationship can be used to estimate the final concentration of contaminants at the water supply well and help in determining the wells susceptibility to contamination.

The incorporation of the Tier 2 model into the susceptibility assessment is the main objective of this study. The model and its application are described in detail in the methodology section of this report.

3. METHODOLOGY

The methodology section outlines the concepts of soil screening models, the formulation of the Tier 2 soil model and its incorporation in the source water susceptibility program. The model is used to compute the reduction in concentration between potential sources of contamination and water supply wells.

3.1 SOIL SCREENING MODELS

Screening models can be described as generic models. These models are based on a simplified interpretation of the natural system, in this case the groundwater system, which enables the development of an analytical solution for the transport problem (Charbeneau and Weaver, 1992). Site-specific models can usually provide a higher level of detail and accuracy than analytical solutions, but they also require the application of numerical methods and detailed site information. The screening models have the advantage of simplicity and require less site-specific information and computation resources.

Many states and regulatory agencies have adopted soil screening models for determining action based decisions at contaminated sites. Soil screening models allow the use of simple models to determine whether the site obtains any risk. Generally, at sites where contaminant concentrations fall below the soil screening levels, no further action is needed. In cases where the screening model determines the site might obtain a risk, more detailed studies or cleanup actions may be needed.

The U.S Environmental Protection Agency (EPA) developed soil screening guidance to help standardize and accelerate evaluations and cleanups of contaminated soils at sites on the National Priorities List (U.S EPA, 1996). This guidance outlines a method for calculating soil-screening levels to evaluate contaminated sites. The model used as the basis for this method is the EPA Composite Model For Leachate Migration with Transformation Products (EPACMTP). This model assesses groundwater quality impacts due to migration of wastes from surface waste sites. The model simulates the transport and attenuation of contaminants from their point of introduction to the water table and within the saturated zone. Applying this model with conservative assumptions and default values together with toxicity information allows the calculation of generic soil screening levels. The Texas Risk Reduction Program uses a similar approach. It uses a tiered approach where generic soil screening levels are determined in the first tier and detailed risk assessments are allowed in the second and third tiers, where more detailed information is available. This approach is described in detail in the following section, especially the Tier 2 model that is incorporated in the source water susceptibility assessment.

3.2 TEXAS RISK REDUCTION PROGRAM – TIERED APPROACH

The Texas Risk Reduction Program applies a tiered approach for evaluating contaminated sites. The most conservative method, in the Tier 1 part, applies pre-calculated general protective concentrations based on general soil and aquifer defaults and toxicity information. The assessment progresses into more

detailed risk assessments in Tiers 2 and 3. Tier 2 and 3 demand site-specific information regarding the soils and aquifer characteristics, while the Tier 1 model is only dependent on the area of the contaminant source.

The Tier 2 model can also fall within the generic model category. Although it utilizes site-specific information, the mathematical formulation is generalized to provide an analytical solution for the groundwater transport problem. This solution provides a more detailed screening model than the Tier 1 model, but the mathematical formulation can still be solved without the use of numerical methods and extensive information is not required. The Tier 2 model also allows the use of general default values where site-specific information is not available. The following figure shows the relationship between the applied model and the information needed.

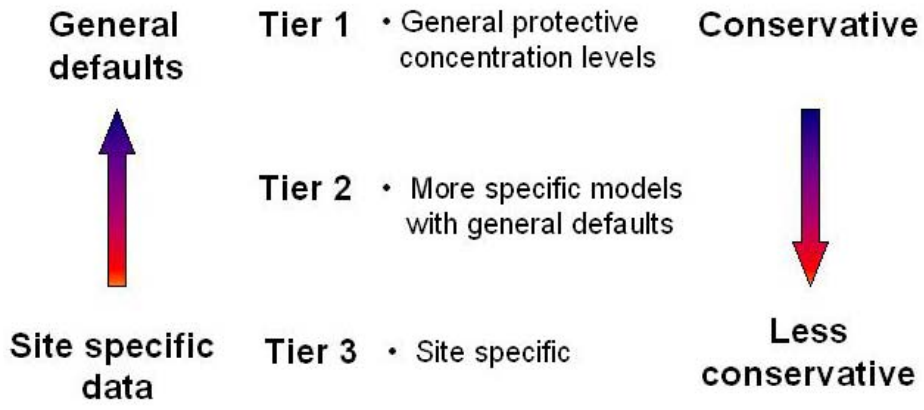

Figure 5 - Tiered approach and information needed

3.3 TIER 2 MODEL

The Tier 2 model described in the Texas Risk Reduction Program (TRRP, Tier 2 PCL Equations) is used in the susceptibility assessment to compute dilution attenuation factors. Using the dilution attenuation factors one can determine the potential of a water source to be contaminated. The model simulates the downward infiltration of contaminants from sources of contamination into the aquifer and then the transport within the saturated zone to the well. The processes simulated by the model include dilution within the aquifer, sorption to soil, dispersion and degradation. A standard linear soil-water equilibrium equation is used to estimate conservative contaminant concentrations in the soil at the source of contamination.

The model is a combination of two separate modules that solve independent parts of the transport problem. The first phase of the model describes the migration from soil to the ground water. This section simulates the mixing of contaminants into the aquifer due to vertical infiltration from the contaminated soil layers above the water table, resulting in a dilution factor. The second phase describes the transport within the saturated zone to the receptor well. This part simulates sorption, dispersion and degradation occurring over this pathway. The result of this section is an attenuation factor that represents the reduction of the concentration due to these processes.

Both pathways are combined to yield a dilution attenuation factor that represents the overall concentration reduction for the complete pathway (from the

contaminated soil to the assessed well). The dilution attenuation factor is combined with a source term to yield a conservative concentration reaching the well from a contaminated site. This relationship is shown in equation 1

$$C_{well} = C_{source} \times DAF \quad (1)$$

where C_{source} is the concentration in contaminated soil at the source of contamination (mg/kg-soil), DAF is the dilution attenuation factor between the source and the well, and C_{well} is the contaminant concentration reaching the well from the source (mg/l). The computed concentrations can be used to estimate the wells susceptibility to contamination. The following section presents the mathematical formulation of the model.

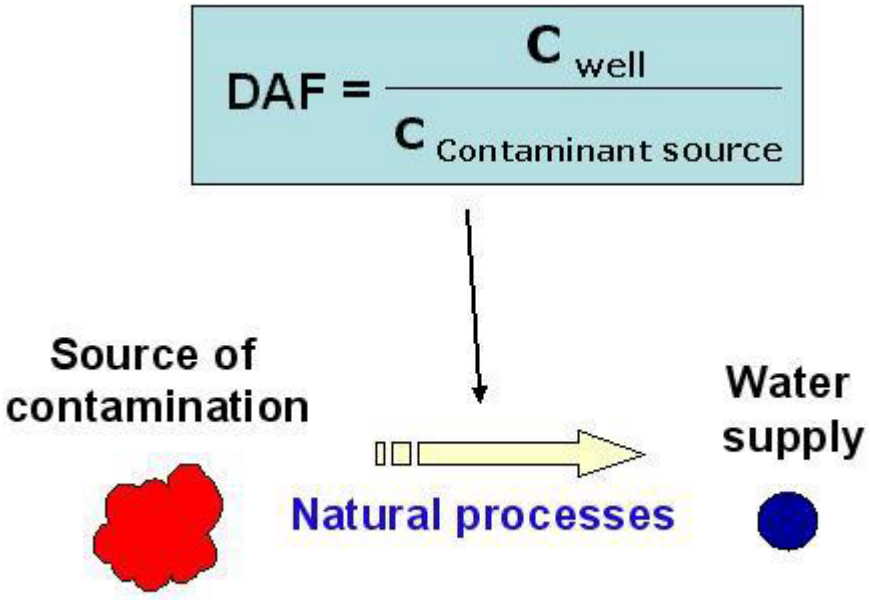

Figure 6 – Relationship between the source of contamination and the supply well

3.4 MATHEMATICAL FORMULATION

The soil screening methodology was designed for use during early stages of site evaluation, when information about the soil and aquifer characteristics is limited. These constraints led to the development of a methodology that is based on conservative, simplifying assumptions simulating the release and transport of contaminants in groundwater systems. The model is described here as two separate pathways and a source term and the simplifying assumptions for each are also presented. The development of the model is described in detail in the EPA soil screening guidance (U.S EPA, 1996). Obviously, any transport model is dependent on soil and aquifer properties as well as the physical-chemical characteristics of the contaminant modeled. In this section a generic model is shown, this model can simulate the transport of any contaminant when the appropriate information is provided. The assembly of a chemical database that holds the appropriate information for the assessed contaminants is described in section 3.5.2.

3.4.1 PHASE 1 – SOIL TO GROUNDWATER PATHWAY

The soil to ground water pathway simulates the dilution of the contaminant infiltrating into the aquifer. This results in a Dilution Factor (DF), which describes the ratio of contaminant concentrations between the groundwater and the soil. The model is based on simple water and mass balances. A basic assumption is the creation of a mixing zone where contaminant concentrations are well mixed and diluted. The horizontal dimensions of the mixing zone depend on the extent of the contaminated site, and its depth is a function of the infiltration

rate and aquifer properties. Figure 6 illustrates the steady-state dilution model where a constant flux of contaminant is introduced into a mixing zone within the aquifer, resulting in a surface of constant concentration at the end of the mixing zone. The concentration from the end of the mixing zone is advectively transported and attenuated during this process.

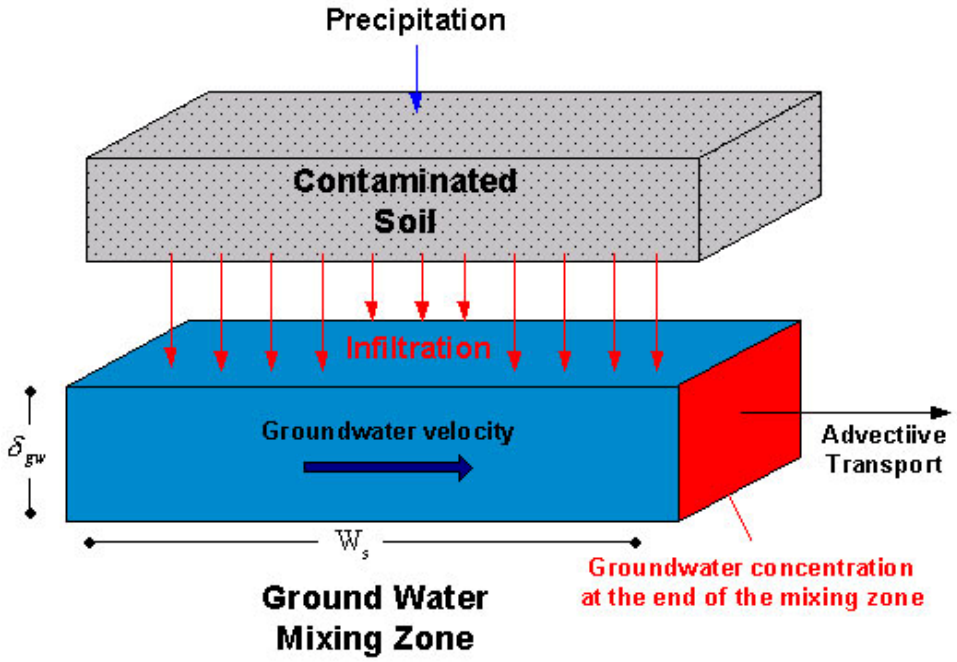

Figure 7 - Dilution of contaminant in the mixing zone

Equation 2 is the governing equation used to calculate the ratio between groundwater concentration, C_{GW} (g/cm^3), and the soil concentration, C_{soil} (g/g-soil). This formula uses the partition equation to estimate the contaminant release from the soil into the water phase and the lateral dilution formula to compute the

concentration after dilution. A description of both formulations is provided in sections 3.4.1.1 and 3.4.1.2.

Equation 2 yields the dilution factor (DF), which is the first term required for the dilution attenuation factor calculation

$$DF = \frac{C_{GW}}{C_{Soil}} = \frac{\left[\dfrac{\rho_b}{\theta_{ws} + K_d \rho_b + H'\theta as}\right]}{LDF} \times \frac{L_2}{L_1} \qquad (2)$$

where ρ_b is the soil bulk density (kg/liter), θ_{ws} the volumetric water content of vadose zone soils (cm^3-water/cm^3-soil), K_d the soil water partition coefficient (cm^3-water/g-soil), H' the Henry's low constant and θ_{as} the volumetric air content of vadose zone soils. L_1 and L_2 are the thickness of affected soil and the depth from the affected soils top to the groundwater table, respectively.

3.4.1.1 Partition equation

The soil-water partition equation is used to estimate contaminant release into soil leachate. The model is based on linear partitioning relations and local equilibrium between the phases of the soil. The local equilibrium assumption allows the expression of the bulk concentration in the soil in terms of a single phase. These relationships can be written with the water phase serving as the reference phase, and the bulk concentration (the mass of constituent per bulk volume) can be written as a function of the soil properties and partitioning properties (Charbeneau, 2000). This assumption allows the calculation of the

concentration in the water phase based on the bulk soil concentration. Eq. 3 shows this relationship where m is the bulk concentration (mg/l-soil).

$$m = (\theta_{ws} + K_d \rho_b + H'\theta as) C_w \tag{3}$$

The bulk concentration can also be expressed as

$$m = C_t \times \rho_b \tag{4}$$

where C_t is the total mass of contaminant in the soil (mg/kg-soil) and C_w the concentration in the water phase of the soil (mg/l). Combining equations 3 and 4 yields the formulation used in equation 5 to represent the contaminant release from soil leachate.

$$\frac{C_w}{C_t} = \frac{\rho_b}{\theta_{ws} + K_d \rho_b + H'\theta as} \tag{5}$$

This equation gives a ratio between the concentration of contaminant in soil and the concentration in the water phase. Using this relationship, in equation 2, the groundwater concentration in the mixing zone can be computed with the soil concentration and the lateral dilution factor.

3.4.1.2 Lateral Dilution Factor

The lateral dilution factor is computed using a simple water balance equation. The calculation assumes the existence of a mixing zone where contaminants infiltrating into the aquifer mix and dilute to create a surface of

constant concentration at the end of the mixing zone (as shown in figure 7). The following equation gives the lateral dilution factor

$$LDF = 1 + \frac{U_{gw}\delta_{gw}}{I_f W_s} \tag{6}$$

where U_{gw} is the groundwater Darcy velocity (cm/year), I_f the net infiltration rate through soil (cm/year), δ_{gw} the ground water mixing zone thickness (meters) and W_s the lateral width of affected vadose zone in direction of groundwater flow (meters).

In the susceptibility assessment the lateral width of contaminated soil (W_s) is estimated as the width of its source. TCEQ has estimated areas of contaminant sources based on the type of the source. Within the water assessment program every point source type is associated with an area, the width is then calculated assuming the source of contamination has a rectangular shape.

The mixing zone depth (δ_{gw}) is estimated with the method used in the EPA Composite Model for Landfills (EPAMCL). The following equation shows the formulation for computing the depth of contaminant penetration, which defines the mixing zone depth

$$\delta_{gw} = (2\alpha_v W_s)^{0.5} + b_{gw}\left[1 - \exp\left(\frac{-I_f W_s}{U_{gw} b_{gw}}\right)\right] \tag{7}$$

where α_v is the vertical groundwater dispersivity (meters), b_{gw} the aquifer thickness (meters) and I_f the net infiltration rate through soil (cm/year).

The first term in this formula, $(2\alpha_v W_s)^{0.5}$, estimates the vertical dispersivity along the travel path underneath the contaminated site. The vertical dispersivity is estimated using an empirical relationship between the vertical and longitudinal dispersivities presented by Gelhar and Axness (1983)

$$\alpha_v = 0.056 \times \alpha_L \tag{8}$$

where α_v and α_L are the vertical and transverse dispersivities. α_L is assumed to be 10% of the flow distance (U.S EPA, 1996). By substituting α_L with 0.1 W_s the transverse dispersivity can be described as,

$$\alpha_v = 0.056 \times \alpha_L = 0.0056\, W_s \tag{9}$$

The second term in the equation, $b_{gw}\left[1 - \exp\left(\frac{-I_f W_s}{U_{gw} b_{gw}}\right)\right]$, estimates the depth due to the downward velocity of infiltrating water.

Theses two terms are added together to estimate the depth of the mixing zone. This depth can also be described as the depth of leachate penetration into the aquifer (Charbeneau, 2000).

Infiltration rates are calculated depending on the soil type. In the Texas risk reduction program three types of soils (sand, silt and clay) are used to calculate infiltration rates as shown in the following equations, which relate the infiltration rate and soil type (TRRP, Tier 2 equations)

Sand $\quad I_f = 0.0018(P)^2 \tag{10}$

Silt $\quad I_f = 0.009(P)^2 \tag{11}$

Clay $\quad I_f = 0.00018(P)^2 \tag{12}$

where I_f is the net infiltration rate through soil (cm/year) and P the mean annual precipitation (cm / year).

Once the lateral dilution factor is computed it can be combined with the partition equation to yield the dilution factor shown in equation 2. The following section describes the general assumptions used in the first phase of the model formulation, the soil to groundwater pathway.

3.4.1.3 Assumptions in the soil to groundwater pathway

Conservative simplifying equations are applied in this pathway to create the analytical solution described above. The following assumptions are used in this phase of the model:

- The model is assumed to be at steady-state, where all variables are constant over time. Emissions from the source of contamination are continuous and result in a constant contaminant concentration in the soil.
- Local equilibrium is assumed between the phases of the soil (water, air and soil).
- The constituent is modeled as being released at the surface. This means that L_2 (the depth from the affected soils top to the groundwater table) is equal to the depth from the surface to the water table.
- The soil contamination extends from the surface to the water table, meaning that the ratio L_2/L_1 is equal to one. Suggesting a conservative approach where the depth of the contaminated soil (L_1) equals the depth from the surface to the water table (L_2). Although this

assumption is conservative, especially in deep aquifers, a separate component (the intrinsic component) of the Texas susceptibility assessment determines the possibility of contaminants reaching the aquifer from the surface. Thus only contaminants that "passed" the intrinsic component test will be assessed in the dilution attenuation component.

- There is no chemical or biological degradation in the unsaturated zone.
- The source of contamination is assumed to have a rectangular shape.
- NAPLs are not present at the site. The method used is applicable for compounds dissolved in the water phase and does not model transport and migration of NAPLs as a separate phase.
- The aquifer is unconfined. Only penetrating sources were assessed for confined aquifers (see section 3.4.6)

3.4.2 PHASE 2 - ADVECTIVE TRANSPORT AND DEGRADATION IN THE AQUIFER

The second phase of the model describes the transport of contaminants in the saturated zone of the aquifer from the end of the mixing zone to the receptor well. The model uses a rectangular surface, with a constant concentration, at the end of the mixing zone as the source term within the aquifer. This concept is demonstrated in figure 8, where the results of the first phase are used as the source term for the second phase of the model.

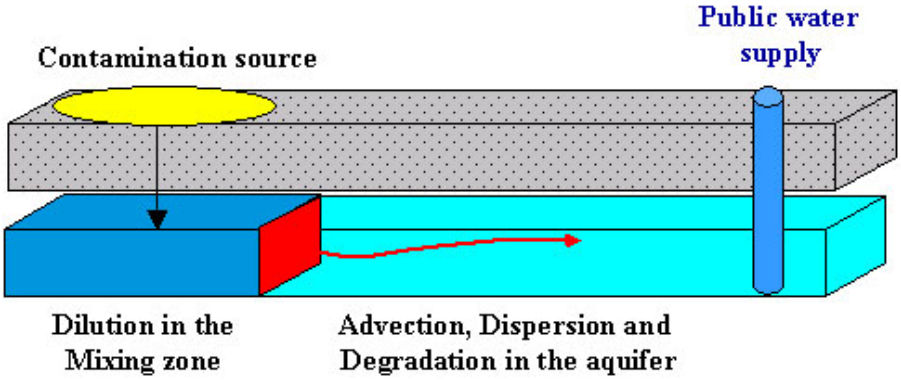

Figure 8 - Transport from the end of the mixing zone to the well includes advection dispersion and degradation

This section of the model simulates advection, dispersion and decay of contaminants in the saturated zone. These processes are modeled to determine the reduction of contaminant concentrations between the end of the mixing zone and the assessed well. The ratio between the concentration at the end of the mixing zone (C_{MZ}) and the concentration at the well (C_{well}) is the Attenuation Factor (AF), this relationship is demonstrated in the following equation

$$AF = \frac{C_{well}}{C_{MZ}} = \exp\left[\frac{L_{GW}}{2\alpha_x}\left(1-\sqrt{1+4\frac{D_g\alpha_x}{v_{COC}}}\right)\right] \times erf\left(\frac{W}{4\sqrt{\alpha_y L_{GW}}}\right) \times erf\left(\frac{D}{2\sqrt{\alpha_z (L_{GW} \text{ or } L_{GW}')}}\right) \quad (13)$$

* *L_{GW}' is used in the vertical dispersivity term when $L_{GW} \geq L_{GW}'$*

where L_{GW} is the down gradient flow distance from the source of contamination to the recipient well (meters), D_g the first order decay constant (day^{-1}), v_{COC} the contaminant retarded velocity (meter/day) and W and D are the source width and depth respectively (meters). α_x, α_y and α_z are the longitudinal transverse and

vertical groundwater dispersivityies (meters). L_{GW}' can be determined from equation 13a.

$$L_{GW}' = \frac{(b_{gw} - D)^2}{\alpha_z} \tag{13a}$$

This is a simplification of the analytical solution for the transport equation of a decaying contaminant (Domenico, 1986). The formulation simulates the advection transport with dispersion and first order degradation. The solution assumes a steady-state case and the equations are simplified to model the centerline of the contaminant plume. Spreading in the vertical direction is allowed only downward, because the source of contamination is assumed to be at the water table.

The retarded velocity of the contaminant can be estimated using the groundwater seepage velocity (v_w) and a retardation factor (R_i) as shown in equation 14.

$$v_{COC} = \frac{v_w}{R_i} \tag{14}$$

The retardation factor is a measure of the velocity difference between solute migration and the water flow. The solute migrates slower than the water because it sorbs onto the soil matrix and has time periods of immobility. Thus, the velocity of a contaminant is lower than the water velocity, depending on the interaction of the contaminant and the soil. Equation 15 is used to compute the retardation factor

$$R_i = 1 + \frac{K_d \rho_b}{\theta_T} \tag{15}$$

where K_d is the soil-water partition coefficient, ρ_b the soil bulk density and θ_T the total soil porosity.

Dispersivities in all directions can be calculated using simple equations derived from estimation models for land disposals regulations, based on field observations (Charbeneau, 2000). The equations estimate the dispersivities as a function of the distance of the transport to the receptor well. The Tier 2 model uses the following relationships between the longitudinal transverse and vertical dispersivities. Equations 16 - 18 show these relationships

$$\alpha_x = 0.1 L_{GW} \tag{16}$$

$$\alpha_y = 0.330 \alpha_x = 0.033 L_{GW} \tag{17}$$

$$\alpha_z = 0.05 \alpha_x = 0.005 L_{GW} \tag{18}$$

where α_x, α_y and α_z are the longitudinal transverse and vertical groundwater dispersivities (meters) and L_{GW} is the down gradient distance from the source of contamination to the well.

The following section describes the general assumptions used in the second phase of the model formulation, the advective transport and degradation within the aquifer.

3.4.2.1 Assumptions in the advective transport pathway

Conservative simplifying equations are applied to create the analytical solution for the pathway described above. The following assumptions are used in this phase of the model:

- The model is at steady-state; all variables are constant over time.
- The depth of the source (D) is set equal to the depth of the mixing zone in the first phase (δ_{gw}).
- The width of the source (W) is equal to the lateral width of affected vadose zone in direction of groundwater flow (W_s) from the soil to groundwater pathway.
- The groundwater velocity for the transport between the mixing zone and the well is computed using the time of travel and the accumulated flow distance. This yields an average velocity over the transport path.
- Soil properties (porosity and bulk density) are constant over the flow path and set equal to soil properties at the source of contamination.

3.4.3 COMPUTING DILUTION ATTENUATION FACTORS

The Dilution Attenuation Factor (DAF) brings together both phases of the model, to give the ratio between concentrations of the contaminant at the recipient well and in the soil at the source of contamination. The DAF is calculated by multiplying the Dilution Factor (DF) and the Attenuation Factor (AF), as shown in the following equation.

$$DAF = DF \times AF \tag{19}$$

The dilution attenuation factor can be combined with a source concentration to estimate a conservative contaminant concentration at the receptor well, as shown in Eq. 1. The source term is presented in the following section.

3.4.4 CONCENTRATION AT THE SOURCE OF CONTAMINATION

The completion of the dilution attenuation factor calculation yields a ratio between the initial contaminant concentration, in the soil at the source of contamination, and the groundwater concentration reaching the recipient well. The next step is to combine the dilution attenuation factor with an initial concentration to estimate the contaminant concentration reaching the receiving well.

The initial concentration in the soil, at the source of contamination, is a function of the physical-chemical properties of the constituent and the soil properties. A conservative method is used to estimate the saturation concentration (C_{sat}). The saturation concentration is the maximum theoretical concentration for a specific contaminant in the soil without creating a non-aqueous phase. To compute the saturation limit the contaminant concentration in the water phase of the soil is set equal to the solubility and local equilibrium between the different phases of the soil (water, air and soil) is applied. Eq. 20 yields the saturation limit as shown

$$C_{sat} = \frac{S}{\rho_b}(\theta_{ws} + K_d \rho_b + \theta_{as} H') \tag{20}$$

where C_{sat} is the theoretical soil saturation limit (mg/kg-soil), S is the solubility of the contaminant (mg/l), ρ_b the soil bulk density (kg/liter), θ_{ws} the volumetric

water content (cm^3-water/cm^3-soil), K_d the soil water partition coefficient (cm^3-water/g-soil), H' the Henry's law constant and θ_{as} is the volumetric air content.

3.4.5 COMPUTING THE CONCENTRATION REACHING THE WELL

The saturation concentration is used as the source term in the model. This term is combined with the dilution attenuation factor to estimate the concentration at the assessed well. The concentration at the source of contamination is set equal to the saturation limit (C_{sat}) and multiplying by the DAF reduces the concentration to simulate the reduction occurring in the transport processes. Eq. 21 is used to estimate the concentration reaching the assessed well.

$$C_{well} = C_{source} \times DAF = C_{sat} \times DAF \quad (21)$$

Both the source term and the dilution attenuation factor are results of conservative methods. These methods are used to compute the maximum effect a potential source of contamination may have on the water supply well.

Concentrations can be calculated for each potential source of contamination that is identified in the contributing area of the assessed well. These concentrations are then used to assess the susceptibility of the well to contamination from point sources.

3.4.6 PENETRATING SOURCES OF CONTAMINATION

Penetrating sources of contamination, which introduce contaminants directly into the water table, are modeled using only the advective phase of the Tier 2 model. Sources such as oil and gas wells, petroleum storage tanks and landfills may penetrate the aquifer and release contaminants directly into the

water table. In these cases the soil to groundwater phase is not applicable and the only reduction in concentration comes from the advective transport phase. The depth of penetration in these cases is set equal to the aquifer thickness and instead of the initial concentration in the soil the solubility of the contaminant is used as the initial concentration at the end of the mixing zone.

The dilution factor in this case can be considered equal to 1 (no dilution) and the following equation is used to calculate the concentration reaching the well.

$$C_{well} = C_{source} \times DAF = Solubility \times AF \quad (22)$$

3.5 DATASETS AND APPLICATION OF THE TIER 2 MODEL

The application of the Tier 2 model utilizes spatial and non-spatial information assembled in the source water assessment program. These sources are combined together using GIS software to extract values from spatial datasets, representing soil and aquifer data, and relating this information with chemical properties and data regarding the potential sources of contamination. Datasets of chemical properties were assembled for the dilution attenuation component of the assessment. Due to the number of constituents assessed in the dilution attenuation component, the range of the contaminants physical properties and the sensitivity of the assessment to the chemical and physical behavior of the constituents in the environment, it is important to utilize detailed information for each contaminant rather than general groupings or common default values to represent the differentiation between contaminants.

3.5.1 SOIL, AQUIFER AND POINT SOURCES DATASETS

Detailed datasets were developed in the source water assessment program to support the susceptibility assessments. These include a variety of spatial datasets for assessing groundwater as well as surface water for the entire state of Texas. In the groundwater point source attenuation component the following spatial datasets were used to calculate the dilution attenuation factor using the Tier 2 model:

3.5.1.1 Soil datasets

Soil properties at the source of contamination are used in the calculation of the dilution factor as well as in the source term, to calculate the saturation concentration in the soil. The soil properties were derived from the State Soil Geographic Database (STATSGO). The STATSGO data comes in vector format and was converted into 60-meter resolution grids. Descriptions of the datasets and the physical meaning of the variables are provided.

- **Soil type** – the soil type categorizes the soils into groups to characterize the soils texture and its physical makeup. Many types and subtypes of soils exist in reality; these are grouped into classes using classification schemes. Standard classifications, such as the USDA standard classification soil texture triangle (Charbeneau, 2000), use the fractions of sand, silt and clay particles in the soil to classify groups. The Texas risk reduction program categorizes the soils into three types, sand, silt and clay. These classes are used in the Tier 2 model to estimate the infiltration rate.

- **Bulk Density** – Bulk density is the ratio of the mass of soil to its total volume (solids and pores together). The units are kg/liter-soil. In the Tier 2 model the bulk density is used to compute the concentrations of contaminants in soil and for computing the retardation factor. The Tier 2 model suggests a default bulk density of 1.67 where no site-specific data is available.
- **Porosity** - Porosity is a measure of the volume of air and water filled pores in the soil. Porosity is a dimensionless (volume/volume) property of the soil; its values can range from 0 in rocks to 0.65 in clays (Charbeneau, 2000). Porosity can also be estimated using equation 23

$$\theta_T = 1 - \frac{\rho_b}{\rho_s} \tag{23}$$

where ρ_b is the bulk density and ρ_s the particle density (g/cm^3). In the Tier 2 model the particle density has a default value of 2.65.

- **Volumetric water content** – Volumetric water content can be described as the fraction of soil pores occupied by water. The volumetric water content is a dimensionless property that can range between 0 and the value of the porosity, when all the pores are filled with water. The Tier 2 model allows the use of a default value, 0.16, when no site-specific data is available.
- **Volumetric air** - The fraction of soil pores occupied by air. Air content is a dimensionless property of the soil. Air content values can range from 0, when the soil is saturated, to the porosity value when

the soil is completely dry. The Tier 2 model allows the use of a default value, 0.21, when no site-specific data is available.

- **Fraction of organic carbon in soil** – The fraction of organic carbon in the soil is used mainly for estimating sorption of organic pollutants to the soil particles. The organic carbon fraction is a mass ratio between the carbon mass and the total soil mass (g-carbon/g-soil). The Tier 2 model allows the use of a default value, 0.002 (0.2%), where no site-specific data is available.

3.5.1.2 Aquifer datasets

Aquifer characteristics are used in the Tier 2 model to compute the dilution attenuation factor. Extensive datasets describing the aquifers in Texas were developed in the source water assessment program. These datasets provide the basis for the groundwater component of the susceptibility assessment. The following datasets were used to execute the Tier 2 model and compute the dilution attenuation factors.

- **Saturated thickness grid** – The saturated thickness is a measure (meters) of the saturated soil within the aquifer. For a confined aquifer the saturated thickness usually equals the aquifer thickness, while for an unconfined aquifer the saturated thickness is less then the aquifer thickness (because of the vadose zone). For the unconfined aquifers the saturated thickness is the difference between the water table/potentiometric surface and the aquifer base. The saturated

thickness is used as the aquifer thickness (b_{gw}) in the dilution attenuation calculation.

- **Darcy velocity grid** – The flow velocity (length/time) is calculated between cells using the Darcy equation that relates the head gradient between the cells to the flow rate. The Darcy velocity is calculated in the delineation process using grids of hydraulic head, porosity and hydraulic conductivity (TNRCC, 1999). The velocity is used in the dilution factor calculation to compute the lateral dilution of contaminants in the aquifer.
- **Time of travel grid** – The time of travel grid is an output of the delineation process. Each cell in the grid has a value that represents the time it takes (years) for water to flow from the cell to the assessed well. The time of travel is used to compute the average flow velocity over the flow path and is incorporated in the attenuation factor calculation.

3.5.1.3 Precipitation information

An average annual precipitation grid is used in the assessment to compute the infiltration rate of water into the aquifer. The infiltration rate is then used in the dilution factor calculation.

3.5.1.4 Potential sources of contamination

Spatial and non-spatial datasets are used to describe the potential sources of contamination. The spatial information identifies the location of the source, to relate it with the contributing zone of assessed wells. The non-spatial information

describes the related contaminants and the source extent. Spatial intersections are used to identify potential sources of contamination within the delineated contributing area of an assessed well. Then specific contaminants can be introduced at these locations, using the relationship between the source type and a contaminant list. As described in section 3.4.1.2 an estimated area for each source type is used to determine the site dimensions.

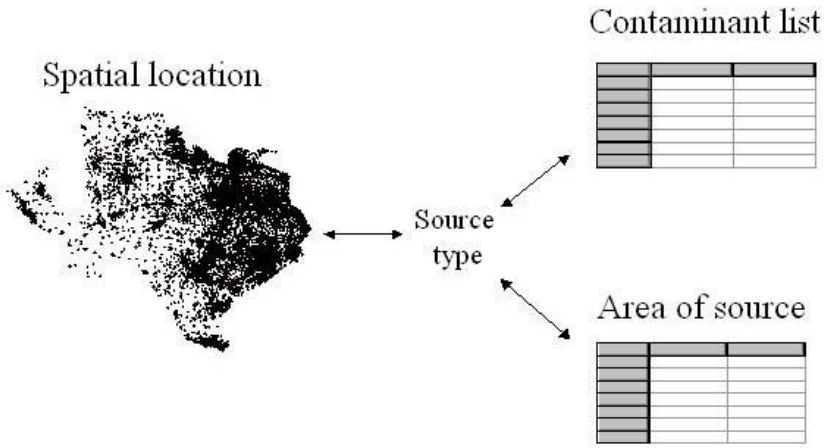

Figure 9 - Using spatial and non spatial information to describe potential sources of contamination

3.5.2 CHEMICAL DATABASE

Physical-chemical properties have a significant impact on the mobilization and degradation of contaminants in the environment. When one models the transport of contaminants and processes such as retardation and degradation it is important to address the variation in chemical properties between the modeled contaminants. In the Tier 2 model a number of physical-chemical properties are required as inputs for the model, these properties were categorized into two classes. The first describes physical properties, such as partitioning coefficients and chemical type and the second class gives its degradation rate.

To support the Tier 2 model a chemical database was established for the dilution attenuation component. The database is developed for all contaminants assessed in the water assessment program. The development process addressed the physical properties and the degradation rates separately using different sources of information and decision rules for each dataset. Each dataset was built from a set of sources that were compiled together, then a set of logical rules were applied to estimate the conservative properties for each contaminant in the database. Conservative properties are the ones that will result in less dilution and attenuation, yielding a higher dilution attenuation factor. Meaning a smaller reduction in concentration occurs during the transport process and the concentration reaching the well will be higher. In soil screening models this will be considered more conservative, due to lower concentrations allowed in the soil at the contaminant source.

The chemical properties required in the dilution attenuation calculation are listed below:

- Type – the type of the constituent (Organic, Inorganic or Metal).
- H - Henry's law constant (unitless or m^3-liq/m^3-air).
- K_d – Soil water partition coefficient (cm^3-water/g-soil).
- K_{oc} – Soil organic carbon partition coefficient (cm^3-water/g-carbon).
- Solubility (mg/l).
- First order degradation rate (1/day).

The list of contaminants and the physical/chemical properties used is described in Appendix 1. A description of the process taken to develop a database with these properties is shown in the following sections.

3.5.2.1 CAS number assignment

The first step in the database compilation was to assign Chemical Abstract Service (CAS) numbers for each constituent. CAS numbers are used as key identifiers in most datasets, literature and computer models. The database compilation started with an initial contaminant list, based on the TRRP PCL table, provided by TNRCC and was completed using SciFinder scholar 2001 software (CAS website). The SciFinder was used where contaminant CAS numbers were missing or where the CAS number was found to be incorrect or to represent an inappropriate form or species of the constituent.

A decision on the contaminant species to be modeled was required in this process. Some contaminants, especially metals, can be present in groundwater in different oxidation states and as either anions or cations. For example, metals are typically modeled in solution in their ionic form and each ion has a different CAS number with different chemical properties. The most common ion or the most mobile form of the metal was usually selected for use in the model. A list of the original contaminants, corresponding CAS numbers, and CAS modifications is provided in appendix 2.

3.5.2.2 Contaminant type

The Tier 2 model categorizes contaminants into three basic groups. These are organics, inorganics and metals. The techniques for selecting or estimating contaminant properties varied among the groups. For example, partitioning of the organic compounds to soil was estimated using local equilibrium/linear partitioning to the organic fraction of the soil. In contrast partitioning of inorganic compounds and metals is often a pH dependent process. As a result, it is necessary to estimate or select pH dependent partition coefficients (U.S EPA, 1996. *Soil Screening Guidance* and U.S EPA, 1996. *Chemical properties for SSL* development).

3.5.2.3 Partition coefficients

The Tier 2 model uses linear partitioning equations and a local equilibrium assumption to relate the concentrations of contaminants in the phases

of the soil. Water is used as the reference phase and the partition coefficients are used to estimate concentrations in the soil and air phases based on the water phase. Partition coefficients are used in the model to calculate the saturation concentration, the soil concentration in the dilution factor and the retardation factor used to estimate the contaminants velocity during the transport in the saturated zone.

The partitioning coefficients that are needed in the Tier 2 model are Henry's law constant, soil water partition coefficient, soil organic carbon and the solubility. These properties were assembled using a variety of sources and a characteristic value was chosen to represent the partitioning of the contaminant. Generally, the most conservative value was chosen to represent the maximum partitioning into the water phase resulting in higher concentrations of the contaminant in the groundwater.

The following section gives a description of the partitioning coefficients and the logical rules applied to select conservative values together with the sources of information used in this process. Varying sources of information were used for organic contaminants vs. metals and inorganic contaminants. The interaction of metals and inorganic contaminants within the environment is highly dependent on environmental conditions such as pH and the water composition. This makes the estimation of partition coefficients for inorganic constituents and metals more challenging.

In cases where no information was available the contaminant was referenced to a similar contaminant for which values were found. In cases where

contaminants are modeled as a group of constituents (i.e. Organotins and PCBs) the constituent with the most conservative partition coefficients was selected to represent the group.

A full list of the partitioning coefficients is presented in Appendices 3 and 4. Different sources of information and methods were used for the organic and inorganic compounds. Appendix 3 shows the organic compounds partitioning coefficients and Appendix 4 gives the coefficients for the inorganic compounds.

Henry's law constant

Henry's law gives a linear relationship between the water and vapor states of a constituent under equilibrium conditions (Charbeneau, 2000). This relationship is expressed using the Henry's law constant, which is shown in equation 24 as the ratio of the vapor pressure to the mole fraction of the substance in the solution.

$$K_H' = \frac{P_{vp}}{X} \tag{24}$$

Where P_{vp} is the vapor pressure (atm) and X is the mole fraction of the substance in solution ($\frac{mole}{m^3}$). The resulting constant has the dimensions of $\frac{atm - m^3}{mol}$. Solubility can be used as an estimate of the mole fraction because it represents the maximum concentration that can be dissolved into the water. The following equation shows this relationship, where the solubility (S) is given in units of mole per cubic meter.

$$K_H' = \frac{P_{vp}}{S} \tag{25}$$

This expression can be normalized using the gas constant (R) and the temperature (T) to yield a non-dimensional Henry's law constant, as shown in equation 26.

$$K_H = \frac{K_H'}{RT} \tag{26}$$

Where R equals $8.2 \times 10^{-5} \frac{atm - m^3}{mol - K}$ and T is the temperature in degrees Kelvin. The non-dimensional Henry's law constant is used in the estimation of mass in the system, using the linear partitioning theory and local equilibrium.

The smallest Henry's law constant was selected to represent smaller partitioning into the air phase resulting in higher concentrations in the water phase of the soil. This leads to higher concentrations of contaminants infiltrating into the aquifer, thus a smaller constant is considered conservative.

Solubility

The solubility of the constituents is used in the source component to estimate the saturation concentration of the soil at the source of contamination. The largest solubility was selected to represent larger partitioning into the water phase resulting in higher concentrations in the water phase of the soil. This leads to higher concentrations of contaminants infiltrating into the aquifer.

Soil water partition coefficients

The methodology used to relate soil and water concentrations is based on linear partitioning. The basic relationship between the soil and water concentrations is shown in the following equation

$$K_d = \frac{C_{soil}}{(C_{water})} \tag{27}$$

where K_d is the linear soil-water partition coefficient (L/kg), C_{soil} the concentration sorbed to the soil (mg/kg) and C_{water} the concentration in solution. The soil water partition coefficient is used in the model to calculate the saturation concentration, the soil partitioning in the dilution factor and the retardation factor in the attenuation factor calculation. K_d values vary significantly by the physical conditions in the soil and different methods are used to derive values for organic compounds and metals, due to varying dominant processes.

For organic compounds the K_d is a function of the hydrophobic character of the compound and the fraction of organic matter present in the soil (Charbeneau, 2000). Equation 28 shows this relationship

$$K_d = K_{oc} \times f_{oc} \tag{28}$$

where K_{oc} is the soil organic carbon partition coefficient (cm^3-water/grm-cabon) and f_{oc} is the fraction of organic carbon in soil (g-carbon/g-soil).

Unlike organic compounds, for which the K_d values can be estimated based on one parameter, the organic matter fraction in the soil. K_d values for metals are affected by a variety of parameters. The most important are pH, oxidation-reduction conditions, iron oxide content, soil organic matter content, cation exchange capacity and major ion chemistry (U.S EPA, 1996).

In order to estimate the K_d one must assume a certain pH. A pH of ***6.8*** was chosen as the typical pH (U.S EPA, 1996 Attachment C) and used to extract specific values from pH dependent information.

The smallest K_d value is selected to represent less sorption to the soil yielding greater mobility of the contaminant and higher concentrations in the ground water. Sorption to soil has a dominant effect on concentrations of degrading constituents. High K_d values will result in a large retardation factor suggesting an immobile contaminant, which will have longer time to degrade before reaching the well.

Sources of information for partitioning coefficients of organic compounds

The following sources of information were used to compile the database for organic contaminants. Partitioning information from the varying sources was compared and the logical rules were applied to select the most conservative value to be used in the Tier 2 model.

- TNRRC Texas Risk Reduction PCL table (TRRP, 30 TAC Chapter 350)
- EPI Suite (EPIWIN V3.10) software was used to retrieve partitioning coefficients of organic compounds. Henry's law constant and sorption coefficients (K_d and K_{oc}) were selected from the Level III Fugacity model inputs. Solubility was extracted from the WSKOW section of the model output.

- Physical Properties Database (PHYSPROP) online Database Demo was used to retrieve Henry's law constants and solubility values.

Sources of partitioning coefficients for metals and inorganic compounds

The following sources of information were used to develop the database for inorganic contaminants and metals. The default pH (6.8) was used when pH dependent information was available.

- TNRRC Texas Risk Reduction PCL table (TRRP, 30 TAC Chapter 350).
- EPA Soil Screening Guidance, User's Guide Attachment C: Chemical Properties for SSL Development (U.S EPA, 1996).
- EPA Soil Screening Guidance, Technical Background Document Part 5: Chemical-Specific Parameters (U.S EPA, 1996).
- EPA Soil Screening Guidance for Radionuclides, Radiological Properties for SSL Development Attachment C (EPA, 2000)
- Environmental Organic Chemistry (Schwarzenbach et al 1993).

Using MINEQL to calculate metals solubility

The solubility of metals varies considerably with changes in the chemical composition of the water, the pH and solid precipitation. Usually metals solubilities are reported using LogC–pH diagrams, which describe the concentration of the metal in the aqueous phase as a function of pH for a given water composition. Solid precipitation is also a dominant process that may determine the aqueous concentration of the metal in solution. In order to model

metals solubility in an aqueous systems one has to take into consideration a variety of factors affecting the metals solubility. This makes the task of determining one characteristic value of solubility very difficult.

To highlight theses difficulties two examples of solubility analysis were processed using MINEQL software. A default pH of 6.8 was used and a background pore water composition was assumed. The examples presented show the variation in the solubility based on changes in the systems characteristics and the chemical interactions considered.

The following water composition (Table 1) was used in the examples. This water composition was used by the EPA in a similar modeling process to determine K_d values for metals (EPA, 1996). The water composition was converted from mg/l to mole per liter, which is required as an input parameter to the MINEQL model.

Parameter	Concentration	
	(mg/l)	(mole/l)
Aluminum	0.2	7.412E-06
Bromine	0.3	3.755E-06
Calcium	48	1.198E-03
Carbonate	187	3.116E-03
Chlorine	15	4.231E-04
Iron(+3)	0.2	3.581E-06
Magnesium	14	5.760E-04
Manganese(+2)	0.04	7.281E-07
Nitrate	1	1.613E-05
Phosphate	0.09	9.477E-07
Potassium	2.9	7.417E-05
Sodium	22	9.570E-04
Sulfate	25	2.602E-04

Table 1 – Background pore water chemistry assumed for the MINEQL simulations (EPA, 1996)

Cadmium and aluminum were selected as examples. Each metal was modeled separately with a concentration of 1 mole per liter as a conservative high concentration of total cadmium or aluminum. pH was set constant at 6.8 and both opened and closed systems were considered for computing total CO_3. An open system suggests that total CO_3 is not a limiting factor in the chemical reactions

because the system is open to the atmosphere. Solubility and complexation data were taken from the MINEQL database (Environmental Research Software, MINEQL+ software).

MINEQL simulation of Aluminum

MINEQL is an equilibrium code. As a result, precipitation of a particular solid phase during a simulation does not consider rates of precipitation. To account for the possibility that the most thermodynamically favorable precipitate may not be the most likely phase to form multiple simulations were performed. The first simulation did not exclude any solid phases from consideration. The model was formulated using a total aluminum concentration of 1M in a closed system. The simulation resulted in precipitation of Diaspore (AlO(OH)). In a second simulation, Diaspore was removed from the active database. In the second simulation precipitation of Gibbsite ($Al(OH)_6^{-3}$) resulted in small concentrations of aqueous aluminum. In the next simulation, gibbsite was assumed to be present in the system and simulations of open and closed systems were preformed to determine the maximum Al concentration in solution at pH 6.8. The total Al^{+3} concentrations are considered as the solubility. The following table shows the total dissolved concentrations from the simulations.

Simulation	Precipitating solids	Fixed solids	Type of system	Total dissolved concentration (M)
1	Diaspore	-	closed	1.27E-9
2	Gibbsite	-	closed	3.34E-8
3		Gibsite	closed	3.34E-8
4		Gibsite	open	3.31E-8

Table 2 - Results of Aluminum modeling with MINEQL

The aluminum precipitants that dominate the system are created by hydroxides and are not dependent on the presence of carbonate. Thus, the open and closed systems simulations were very similar. Systems with hydroxide precipitants are dominated by variations in pH. The following LogC-pH diagram shows the change of total dissolved aluminum as a function of pH.

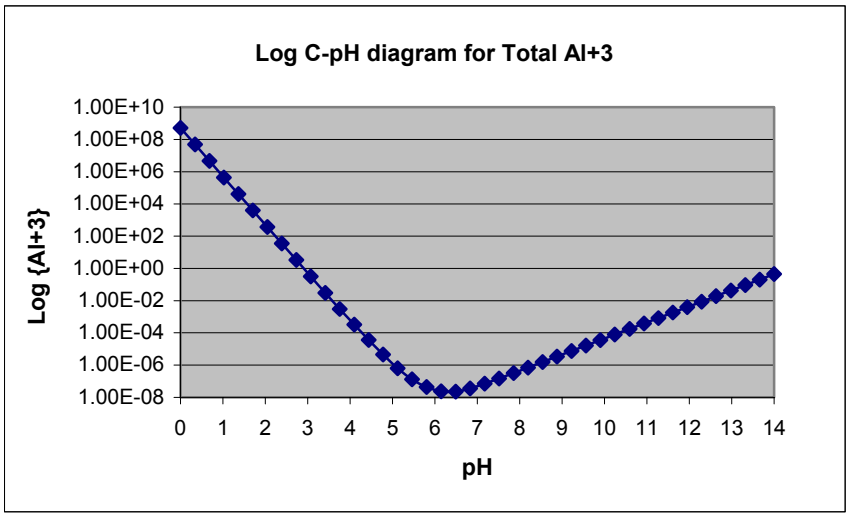

Figure 10 - LogC-pH diagram for total Al^{+3}

The above diagram shows the sensitivity of the Al^{+3} dissolved concentration to pH variation. The changes in the solubility with variations in pH can be on orders of magnitude, making it difficult to predict a specific solubility.

MINEQL simulation of Cadmium

The second simulation set modeled the interaction of 1M total cadmium added into the system. The first simulation of a closed system did not result in any precipitation of solids and over 99% of the cadmium remained in solution. This suggests that the solubility (equal to the total dissolved concentration) is dominated by the initial input of Cd^{+2} into the system. Two open system simulations were preformed and the partial pressure of CO_2 was varied (to run the simulations $Cd_3(PO_4)_2$ and $Cd_4(OH)_6SO_4$ were removed from consideration). These simulations resulted in much lower dissolved concentrations of cadmium due to Otavite ($CdCO_3$) precipitation. These simulations show the sensitivity of the cadmium system to carbonate. Another simulation with fixed $CaCO_3$ was preformed to simulate the interactions in calcareous formations, which may be a source of carbonate to groundwater systems. The following table shows the dissolved concentrations from the simulations.

Simulation	Precipitating solids	Type of system	Total dissolved concentration (M)
1	None	closed	0.996
2	Otavite	Opened (LogPCO2 =-3.5)	1.6E-4
3	Otavite	Opened (LogPCO2 =-1.5)	1.68E-6
4	Otavite	Closed, Fixed $CaCO_3$	3.1E-4

Table 3 - Results of Cadmium modeling with MINEQL

The above results show the variation in cadmium solubility with respect to carbonate availability. The more carbonate available in the system, more solid precipitates and the lower the solubility. The interaction of cadmium within the groundwater systems will depend on the carbonate available from the atmosphere or the geological formations.

The examples shown for aluminum and cadmium highlight the difficulty of modeling metals interactions within groundwater systems. Solubility may vary by orders of magnitude depending on the water composition, the pH of the system and the precipitation of solids. Using a single value of solubility to model metals transport through groundwater systems will not be accurate. A better approach

might use a number of solubility values depending on the aquifer water composition, pH and rock formation.

3.5.2.4 Degradation rates

Degradation rates have a major impact on the results of the dilution attenuation component. Degradation half-lives represent a range of individual processes that decrease the contaminant concentration over time. These processes can be related to microbiological processes, such as aerobic and anaerobic biodegradation, or to physical-chemical processes such as hydrolysis, photolysis oxidation-reduction processes and radiological decay. All these processes have to be addressed to result in one overall half-life.

Degradation rates reported in literature are highly variable, depending on the source of information. A conservative approach was taken, meaning the lowest degradation rate (longest half life) found was selected, resulting in higher concentrations of the contaminant for longer travel distances in the aquifer. The following sources of information were used to develop the degradation rate database. The full list of degradation rates is presented in appendix 5 for organic compounds and in appendix 4 for inorganic compounds.

Sources of degradation rates for organic compounds

- Handbook of Environmental Degradation Rates (Howard et al, 1991).

  This book presents overall half lives for many of the assessed contaminants. The book gives a range of values rather than showing a single half live value. The smallest half life was chosen as the conservative value.

- EPI Suite (EPIWIN V3.10)

The Level III Fugacity section of the EPI model was used to determine half-lives of organic compounds. The EPI Suite model gives the half-lives in surface water. Howard et al (1991) suggest that biodegradation and hydrolysis, to a lesser extent, are the principal means of degradation. They also recognize that biodegradation in groundwater proceeds at a slower rate compared to surface water. To account for this difference degradation rates in groundwater were taken as half the degradation rate in surface water, unless other information was available.

The half-lives from the available sources were given in hours, these selected half-lives were converted into degradation rates by applying the following equation that relates the degradation rate to the half-life of contaminants

$$D_g = -\frac{\ln(0.5)}{24 \times T_{1/2}} \tag{29}$$

where D_g is the first order degradation rate (day^{-1}) and $T_{1/2}$ the half-life of the constituent (hours).

Sources of degradation rates for metals and inorganic compounds

Degradation rates for metals and most of the inorganic compounds were set to zero, in most cases these compounds do not degrade but change forms due to chemical reactions. For a number of the metals and the radioactive elements, half-lives were obtained from: the following sources:

- EPA Soil Screening Guidance for Radionuclides, Radiological Properties for SSL Development Attachment C (EPA, 2000)
- EPA Soil Screening Guidance, User's Guide Attachment C: Chemical Properties for SSL Development (U.S EPA, 1996).
- Oak Ridge Reservation Annual Site Environmental Report 2000, Appendix G (ASER, 2000).

  This report was used only for the degradation rate of Strontium 89.

3.5.3 MODEL APPLICATION USING GIS

An application to calculate dilution attenuation factors from point sources of contamination to water supply wells was created using ArcGIS and Microsoft Access databases. The ability of ArcGIS to combine spatial information and tabular datasets and the simple linkage between it to relational database programs provides an adequate environment to execute this type of assessment.

The mathematical formulation is solved in one Microsoft Access database that assembles all the information necessary from the spatial and non-spatial datasets. The assembled databases and flow of information is shown in figure 11.

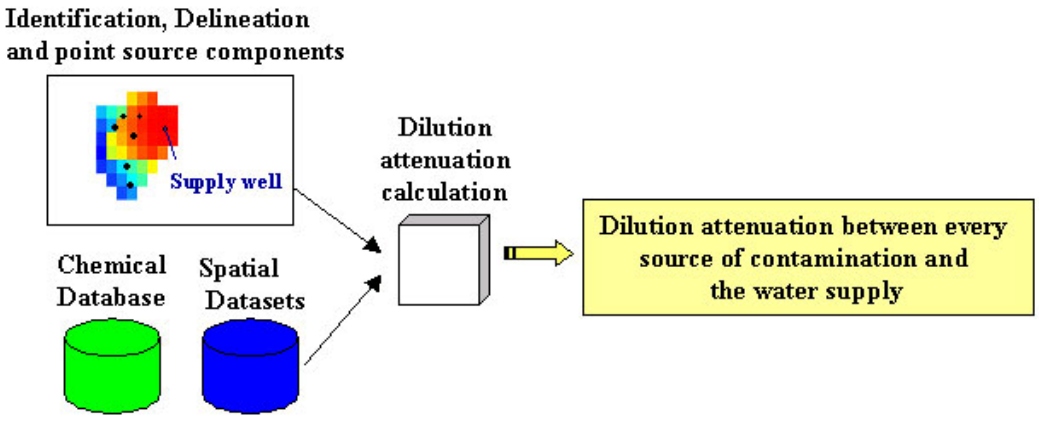

Figure 11 - Model application using GIS

The following spatial and non-spatial querying procedures are needed to calculate the dilution attenuation factor from every source in the capture zone of the water supply well:

- Spatial datasets are queried based on the sources spatial location to extract soil and aquifer properties as well as precipitation rates for each source.
- Each source is associated with an area and a contaminant list in the point source component.
- Contaminants are related to chemical properties by querying the chemical database.

Once all information is assembled into the calculation table, the Tier 2 model application calculates a dilution attenuation factor from each potential source to the assessed water supply well for all contaminants related to the sources in the capture zone.

3.5.4 APPLICATION EXAMPLE FOR ONE WELL

An example of the model's application for one well is presented to demonstrate the computation of the dilution attenuation factor and the aggregation of the results to determine overall susceptibility. In the example, one well is assessed for one contaminant. Benzene was selected as the contaminant of concern in the example. Table 4 presents the chemical properties of Benzene used in the example.

Chemical property	Units	Value
Chemical Type	-	Organic
Henry's Law constant (H)	Unitless	0.227
Soil organic carbon – water partition coefficient, Log(Koc)	cm^3-water/g- carbon	1.74
Degradation Rate (Dg)	1/day	1.671E-06
Solubility (S)	mg/l	2,000

Table 4 – Chemical properties of benzene

The first step in assessing the susceptibility of the well is to identify the potential sources of contamination within its contributing area. The following image shows the assessed well and 5 potential sources of benzene identified in its capture zone (this is the outcome of the identification and delineation components).

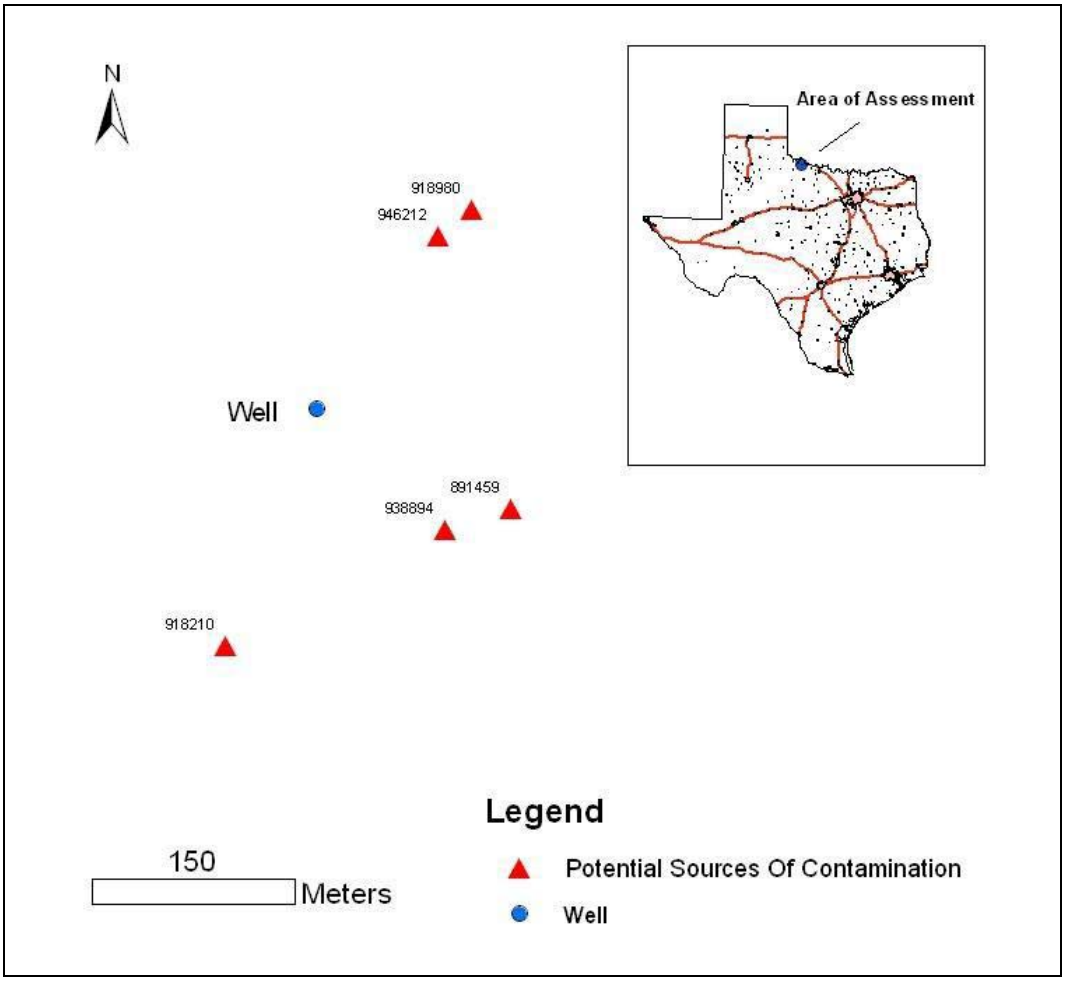

Figure 12 - Assessed well and Benzene potential sources of contamination

Once potential sources of contamination are identified, the types of the sources their area and soil and aquifer properties are extracted from the spatial datasets and the area of the contamination sources are estimated. Tables 5 and 6 present the source, soil and aquifer properties of the identified sources of contamination.

Source ID	Penetrating code	Area	Bulk density	foc	soil type	Volumetric air content	Volumetric water content	Precipitation
	0 = not penetrating -1 = penetrating	sq. meters	Kg/liter	g-carbon/g-soil				cm/year
891459	0	1000	1.1716	0.27	Silt	0.21	0.6456	65.7
918210	0	1000	1.1716	0.27	Silt	0.21	0.6456	65.7
918980	0	1000	1.1716	0.27	Silt	0.21	0.6456	65.7
938894	0	1000	1.1716	0.27	Silt	0.21	0.6456	65.7
946212	0	1000	1.1716	0.27	Silt	0.21	0.6456	65.7

Table 5 - Source and soil properties

ID	Aquifer Thickness	Flow Distance	Time of travel	Darcy Velocity at the source of contamination
	meters	meters	days	cm/year
891459	5.5	205	234	21554
918210	6.1	205	119	42769
918980	4.9	170	423	7645
938894	5.8	170	116	30773
946212	4.9	170	423	7645

Table 6 - Aquifer and flow properties

Equation 9 is used to compute the vertical dispersivity (α_v) and equations 10 to 12 for calculating the infiltration rate (I_f). Then substituting these properties into equation 7 yields the mixing zone depth (δ_{gw}). These values are used in equation 6 to yield the lateral dilution factor (LDF). Then the dilution factor is computed using equation 2, the LDF and the soil and chemical properties. Table 7 shows the dilution factor calculation for the 5 potential sources of contamination.

ID	I_f	α_v	δ_{gw}	LDF	DF
	cm/year	meters	meters		
891459	3.890	0.177	3.352	5.88E+02	1.10E-04
918210	3.890	0.177	3.350	1.17E+03	5.55E-05
918980	3.890	0.177	3.363	2.10E+02	3.08E-04
938894	3.890	0.177	3.351	8.39E+02	7.71E-05
946212	3.890	0.177	3.351	8.39E+02	7.71E-05

Table 7 - Dilution Factor (DF) calculation results

The second phase is the calculation of the attenuation factor. The first step in the attenuation factor computation is to calculate the groundwater seepage velocity from the time of travel and the flow distance. The retardation factor is then computed using equation 15, the K_d of the contaminant and the soil properties. For organic compounds the K_d is derived from K_{oc} and foc as shown in equation 28. Then the retarded velocity of the contaminant can be estimated with equation 14 and the retardation factor. To complete the inputs needed for the AF calculation the longitudinal vertical and transverse dispersivities are calculated with equations 16-18. The width of the source (W) is set equal to the sources width from the DF calculation and its depth (D) is equal to the depth of the mixing zone (δ_{gw}) from the DF calculation.

Substituting these properties into equation 13, together with the degradation rate and the flow distance yields the Attenuation Factor (AF). Table 8 shows the results of the attenuation factor calculation.

ID	L_{GW}	α_x	α_y	α_z	V_w	Ri	V_{coc}	W	D	AF
	meters	meters	meters	meters	meter/day		meter/day	meters	meters	
891459	205	20.5	6.8	1.0	0.878	59.09	0.015	31.62	3.35	1.69E-01
918210	205	20.5	6.8	1.0	1.724	59.09	0.029	31.62	3.35	1.43E-01
918980	170	17.0	5.6	0.9	0.402	59.09	0.007	31.62	3.36	2.40E-01
938894	170	17.0	5.6	0.9	1.465	59.09	0.025	31.62	3.35	1.87E-01
946212	170	17.0	5.6	0.9	0.402	59.09	0.025	31.62	3.35	1.87E-01

Table 8 - Results of the Attenuation Factor (AF) calculation

The final Dilution Attenuation Factor (DAF) is calculated by multiplying the dilution and attenuation factors as shown in equation 19. A conservative concentration estimated to reach the well is calculated using the saturation limit as the source term and the DAF. The saturation limit formula is given in equation 20 and is based on soil and chemical properties. The concentration estimated to reach the well is calculated using equation 21. Table 9 shows the computation of the DAF and the concentration reaching the well.

ID	DF	AF	DAF	C_{sat}	C_{well}
				mg/liter	mg/liter
891459	1.10E-04	1.69E-01	1.86E-05	3.09E+04	5.75E-01
918210	5.55E-05	1.43E-01	7.91E-06	3.09E+04	2.45E-01
918980	3.08E-04	2.40E-01	7.38E-05	3.09E+04	2.28E+00
938894	7.71E-05	1.87E-01	1.44E-05	3.09E+04	4.45E-01
946212	7.71E-05	1.87E-01	1.44E-05	3.09E+04	4.45E-01
				Average concentration	**7.98E-01**

Table 9 - Results of the DAF and concentration calculations

The overall susceptibility estimated for the well is an aggregation of all the concentrations calculated for the individual sources of contamination. In the Texas source water assessment program the average concentration is used to estimate the susceptibility of the well. The average concentration is compared to water quality thresholds, determined by TCEQ, to evaluate the wells susceptibility. For example an average concentration smaller than the threshold will be considered as low, between the threshold and half the water quality standard will be medium and concentrations above half the water quality standard will be high.

The water quality threshold used for benzene in the Texas source water assessment program is 1E-4 mg/l and the water quality standard is 5.0E-03 mg/l. Comparing the average concentration shown in table 9 with the water quality thresholds, the susceptibility of the well to Benzene contamination is determined as high (the estimated concentration is larger then the water quality standard).

4. RESULTS

The dilution attenuation component results in a set of conservative concentrations computed for each potential source of contamination in the contributing zone of the assessed well. The concentrations can be aggregated using various methods to yield one concentration expected at the well. These are used to determine the susceptibility of the well to contaminants. The higher the predicted concentration, the more susceptible the well is to contamination.

A variety of physical properties influence the susceptibility of wells to contamination. These include the presence of sources of contamination in the vicinity of the well as well as the properties of the aquifer in which the well is screened. To try and understand the relationships between the aquifer properties, contaminant sources and the susceptibility of the well, spatial trends were examined and compared with water quality monitoring information. The following sections give examples of methods and processes that can be used to help determine the susceptibility of water supply wells.

4.1 COMPARISON OF THE DILUTION ATTENUATION RESULTS WITH WATER QUALITY DATA

The dilution attenuation results were compared with a water quality database to study the accuracy of the model in capturing water quality problems. As described above, the Tier 2 model yields a conservative estimation of pollutant concentrations reaching a well from each source of contamination. The

aggregation of these results gives an estimate of the susceptibility of the well to contamination. These results are compared to water quality samples taken at public water supplies.

TCEQ compiled a water quality database (the "Master Chemical list") that shows water quality monitoring results at public water supplies. This database gives information at a specific entry point of the water supply system, where the samples were taken. The database includes about one million records of monitoring data at over 10,000 entry points for 159 contaminants. These monitoring points may receive water from a number of wells, thus it is difficult to make conclusions on the origin of the contaminant measured at the monitoring point. The following image illustrates this difficulty.

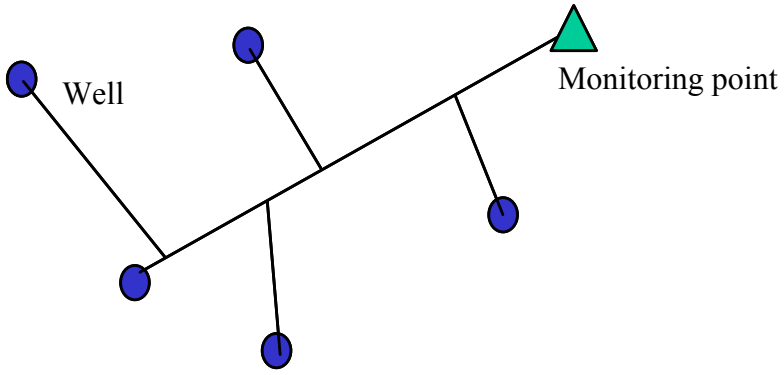

Figure 13 - Wells contributing to a monitoring point on the water supply network

Another water quality database used in the comparison is the "Finished Water" database, compiled by TCEQ from the "Master Chemical List" and used in the source water assessment program. In this database water quality measurements from the "Master chemical list" were compared to a threshold, determined by TCEQ, and all observations that exceeded the threshold were

included in the dataset. Due to the difficulty in relating the detection to a specific well, all wells that contribute to that monitoring point were treated as contaminated and were included in the database. The result of this process is a list of wells in which specific contaminants have been detected. The "Finished Water" database includes over 85,000 wells related with 124 contaminants at over 5,500 public water supplies.

Three groups of contaminants are selected for the comparison, BTEX compounds (Benzene, Toluene, Ethylbenzene and Xylenes), PCE (Tetrachloroethylene) and PCE daughter products (TCE, 1,1-DCE, 1,2-DCE, Vinyl Chloride) and MTBE (Methyl-T-Butyl Ether). These contaminants were selected because they are generally related to point sources of contamination. The dilution attenuation component models only point sources of contamination. To minimize the influence of non point sources, these groups of contaminants that are likely to arise from point sources of contamination, were selected for the comparison.

Water quality measurements from the "Master chemical list" database were compared with a series of thresholds ranging from the detection limit to water quality standards. Each water quality sample is compared to the threshold and assigned a yes/no value for exceeding or not exceeding the threshold. The positive results of the comparisons were then aggregated by the public water supply, resulting in a list of water supplies with at least one detection that exceeds the threshold. The following table presents the thresholds and water quality standards used for the comparison.

Contaminant	CD*	Group	Threshold = Detection limit		Water quality standard	
			mg/l	Microgram/l	mg/l	Microgram/l
BENZENE	56	BTEX	0.0001	0.1	0.005	5.0
ETHYLBENZENE	125	BTEX	0.0001	0.1	0.700	700.0
TOLUENE	211	BTEX	0.0001	0.1	1.000	1000.0
XYLENES (TOTAL)	226	BTEX	0.0001	0.1	10.000	10000.0
METHYL-T-BUTYL ETHER	159	MTBE	0.0001	0.1	0.244	244.4
1,1-DICHLOROETHANE	5	TCE	0.0001	0.1	2.444	2444.2
1,2-DICHLOROETHANE	12	TCE	0.0001	0.1	0.005	5.0
TETRACHLOROETHYLENE	208	TCE	0.0001	0.1	0.005	5.0
TRICHLOROETHYLENE	219	TCE	0.0001	0.1	0.005	5.0
VINYL CHLORIDE	225	TCE	0.0001	0.1	0.002	2.0

** CD is a unique identifier used in the Texas Source Water Assessment Program*

Table 10 - List of contaminants used in the comparison, their threshold and water quality standard

The results from the aggregation of water quality detections were then compared to the estimated concentrations computed using the Tier 2 model. The following table shows the results obtained from this comparison when the threshold was varied between the detection limit and the water quality standard.

Threshold		Water supplies with detections above the threshold	Supplies with detections above the threshold and sources of contamination identified	% of supplies with detections that have contaminant sources
	Microgram/l			
Detection limit	0.1	1547	505	32%
Detection limit × 10	1	1053	348	33%
Detection limit × 100	10	154	60	38%
Water quality standard	Contaminant dependent	39	13	33%

Table 11 - comparison of the number of water supplies with detections and the number of water supplies with identified sources of contamination

The above table shows that only up to 38% of the public water supplies that had water quality detections of BTEX, PCE compounds or MTBE actually had sources of contamination identified within their capture zone. The implications of this result is that if one tried to predict where water quality problems might occur by looking at the contamination sources, only up to 38% of the occurrences would be predicted. This estimation only looks at the occurrences of contaminant sources within the capture zone of the well without using the reduction of concentration modeled by the dilution attenuation component. Thus,

the estimation is less conservative if the dilution attenuation component is used the accuracy of the predictions will be lower.

4.2 EXTRACTING SPATIAL TRENDS FROM THE RESULTS

Spatial trends of susceptibility can be observed by aggregating and interpolating the results computed for each well in the dilution attenuation component. The susceptibility of a water supply can be correlated with a variety of attributes, which can roughly be categorized into two categories. The first is the presence of contamination sources, which determine what potential contaminants are in the area of the water supply and where these contaminants are introduced into the environment. The second category includes the aquifer properties, which determines the likelihood that the contaminants introduced to the environment will reach the wells and at what magnitude.

The following sections show examples of spatial trends that can be used to study susceptibility patterns. These trends include distributions of contaminant sources and wells and the characteristics of the aquifers assessed.

4.2.1 ANALYSING SOURCES OF CONTAMINATION USING SPATIAL FUNCTIONS

The density function in ArcGIS spatial analysis was used to extract the density of potential sources of contamination for each chemical group. Mapping density highlights the areas of higher concentration of features. It is especially useful in areas with many features where it is hard to identify trends by simple

mapping of the features (Mitchell, 1999). The following maps illustrate the advantage of density maps vs. simple mapping of features.

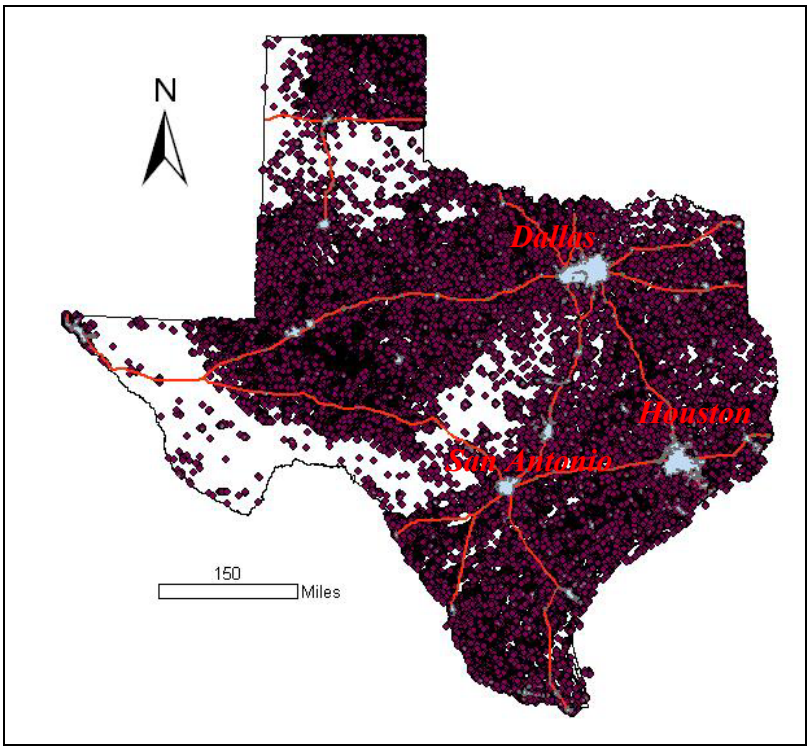

Figure 14 - Potential sources of contamination for BTEX compounds

From the above map it is apparent that spatial trends are hard to extract in areas where many features are located. In order to better understand the spatial trends a density map of the features is created. Using the map below one can understand the relative spatial trends and distribution of BTEX sources. These types of maps can be used to estimate the potential for contamination from the different contaminants based on the occurrence of sources in the water supplies vicinity.

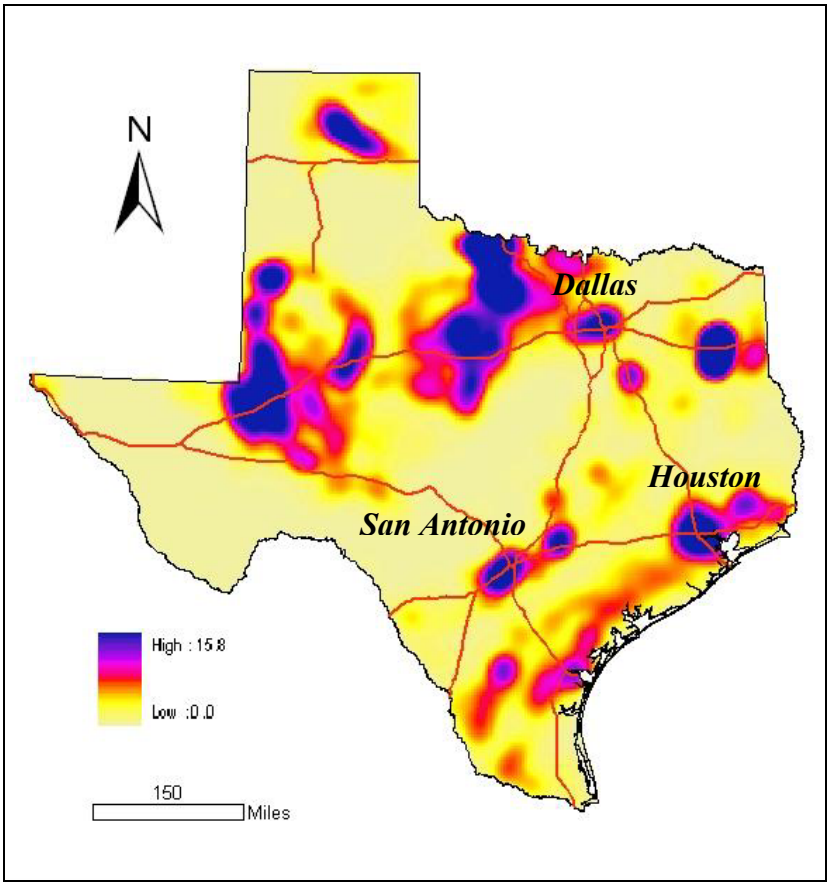

Figure 15 - Density (number of sources per square km) of potential sources of contamination for BTEX compounds

The density map shows a correlation between the urban areas and the number of potential sources of contamination for BTEX compounds. A similar correlation can be noticed with TCE and its degradation products (referred to as the TCE group of compounds) where high densities of sources are correlated with large metropolitan areas such as Dallas, Houston and San Antonio. Figure 16 shows this correlation.

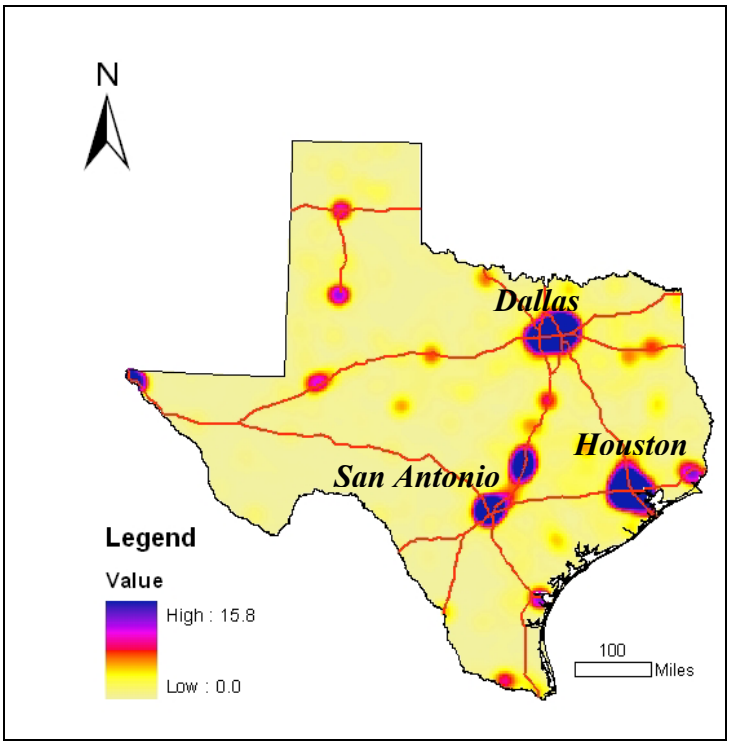

Figure 16 - Density of potential sources of contamination for TCE group compounds (sources per square km)

4.2.2 CORRELATION BETWEEN DENSITY OF CONTAMINANT SOURCES, WELL DISTRIBUTION AND WATER QUALITY DETECTIONS

Using the density maps to describe the source of pollutants into the environment one can try to find a correlation between the presence of contaminants in high density areas of contaminant sources and water quality observations. The following map shows this relationship between the water quality detections and the density of the contaminant sources.

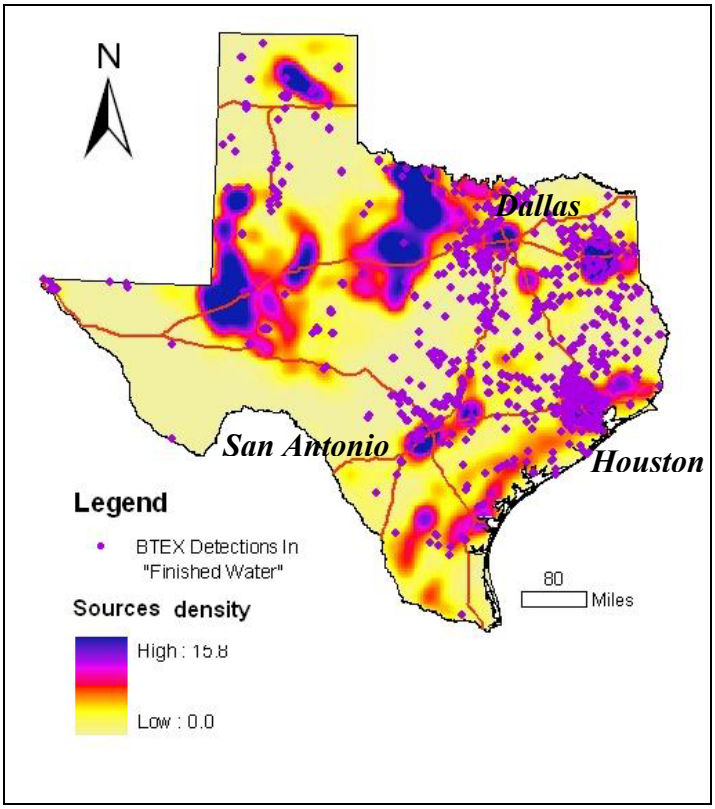

Figure 17 - BTEX measurements above the detection limit (0.1 microgram/l)

Figure 17 shows the BTEX detections that exceeded a threshold of 0.1 microgram per liter on top of the density of BTEX sources of contamination. The detections are based on the "Finished Water" water quality database described in section 4.1. The development of the density map is shown in Figures 15 and 16.

The map in Figure 17 shows that the majority of detections are in areas of high density of contaminant sources. Still there are large areas that show high density of contamination sources but have few water quality detections. This can be explained by the following map, which displays the water quality detections together with the spatial distribution of wells.

Figure 18 shows BTEX detections from the "Finished Water" database over the density of water supply wells. It is clear from the map that a majority of detections are found in areas with high densities of wells. The absence of detections in some areas with high densities of contaminant sources observed in figure 17 can be attributed to the absence of wells in those areas. Generally, where there are no wells there is no need for monitoring, thus contaminants will not be detected.

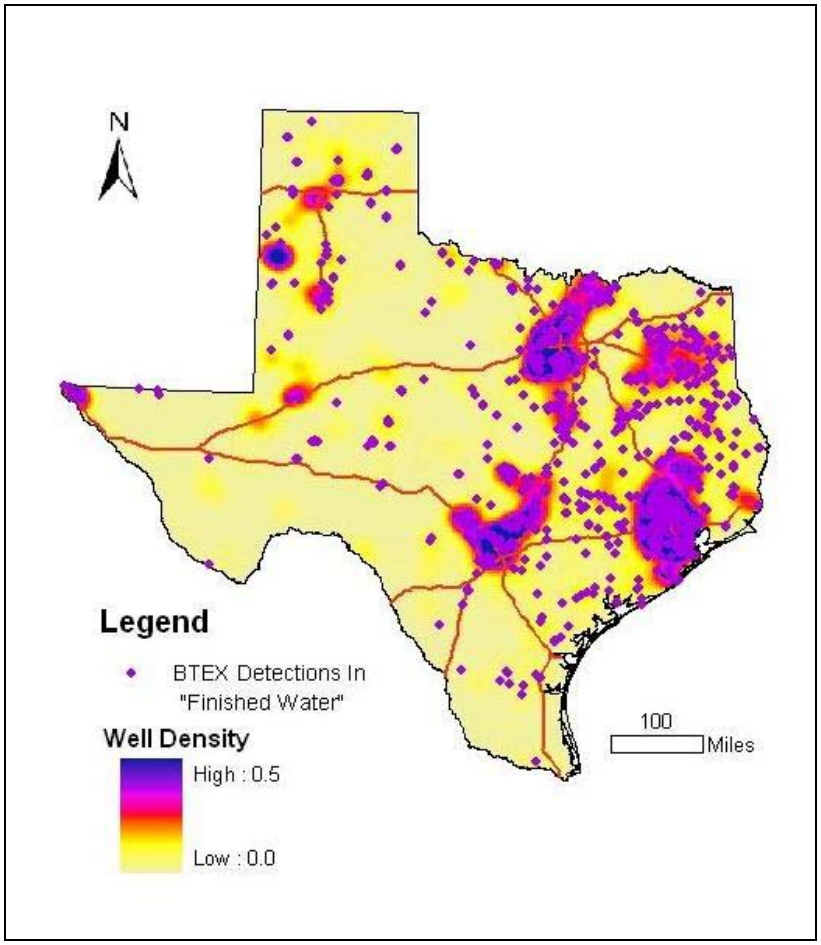

Figure 18 - BTEX detections compared with well density

Figure 19 shows a similar case for TCE and its degradation products, where the water quality detections fall within dense areas of wells. These maps demonstrate the combination of factors that influence water quality. Characteristics such as the density of wells may contribute to water quality deterioration when combined with contaminant source occurrences. Another alternative is that where large numbers of wells exist, more detections will be observed based on the larger sampling space that increases the probability to observe detections.

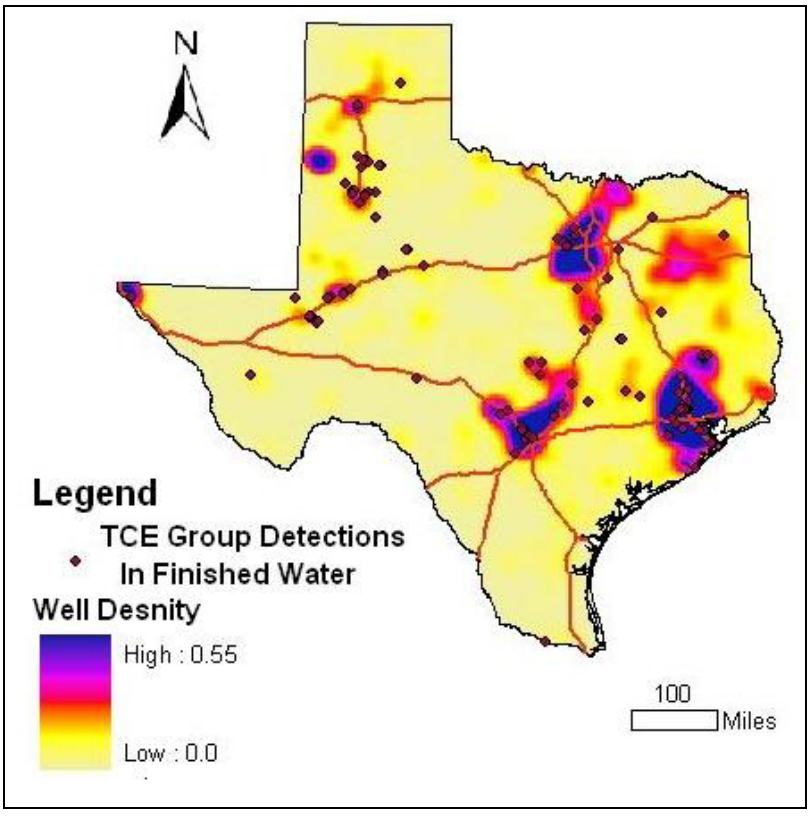

Figure 19 - TCE group detections compared with well density

When analyzing these maps one must use caution because the construction of the "Finished Water" database may create trends in the data that are not realistic. In the database, all wells contributing to a sampling point with one or more detections are considered contaminated. This may result in multiple detections where only one detection actually exists. In order to insure the trends seen in the above maps are realistic the "Finished Water" database was aggregated by the public water supply and only one well from that water supply was assumed contaminated. The following maps show the results of the aggregation by water supply for the BTEX and TCE groups of contaminants.

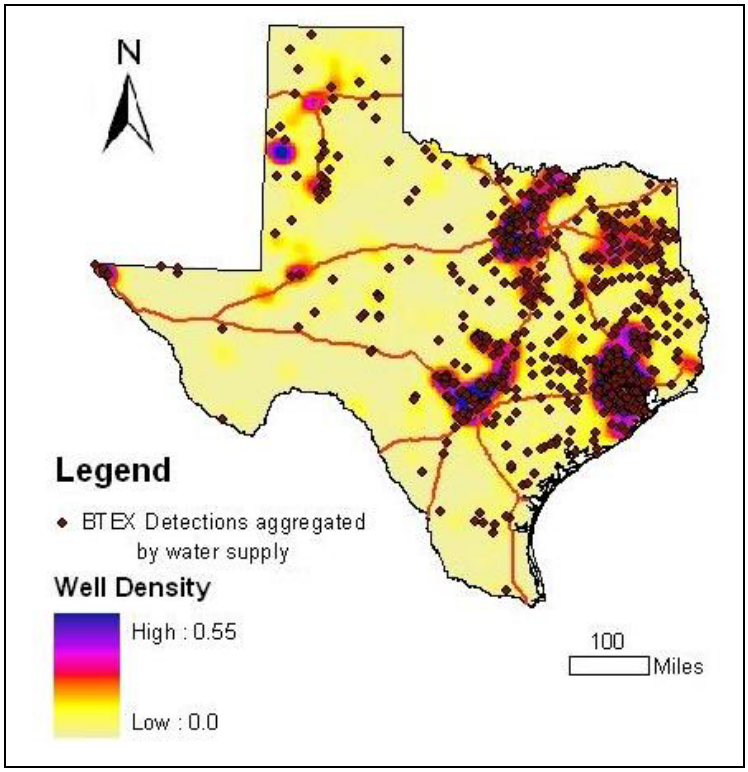

Figure 20 - BTEX detections aggregated by water supply compared with density of wells

Figure 20 shows that the aggregation by water supply resulted in a similar distribution of water quality detections as when all wells in the water supply were treated as contaminated. The following map illustrates the same result for TCE compounds.

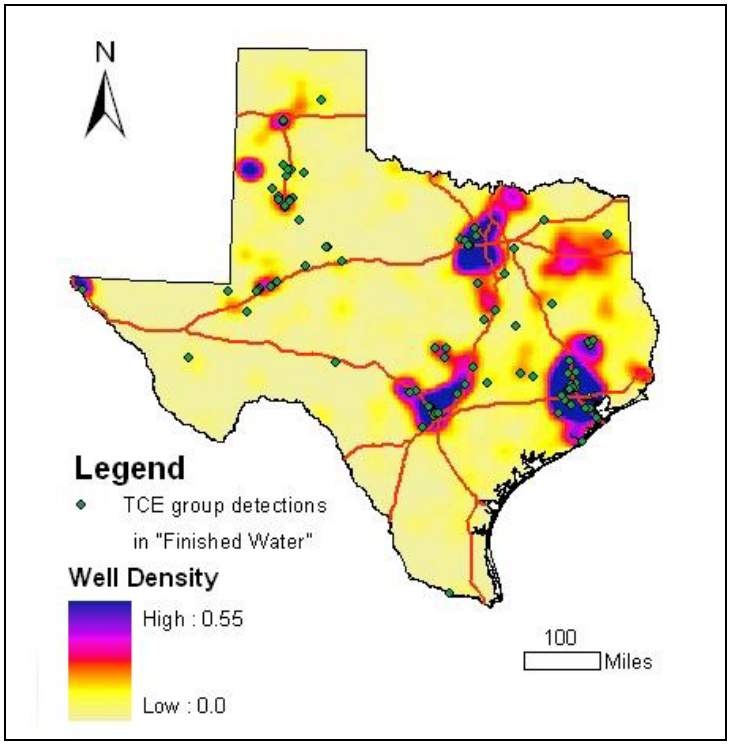

Figure 21 - TCE group detections aggregated by water supply compared with well density

The similar distribution of water quality detections in both cases suggests the use of the "Finished Water" database in its original form is reasonable for the contaminants assessed. Although the distribution of the detections is similar a closer look at the magnitude of detections, or the density of detections in a certain area, may be significantly different between the aggregation methods. A single

detection measured at a monitoring point related to many wells may result in high density of detections due to the assignment of the contaminant to all the wells. The following maps show the densities of BTEX detections for both methods of aggregation.

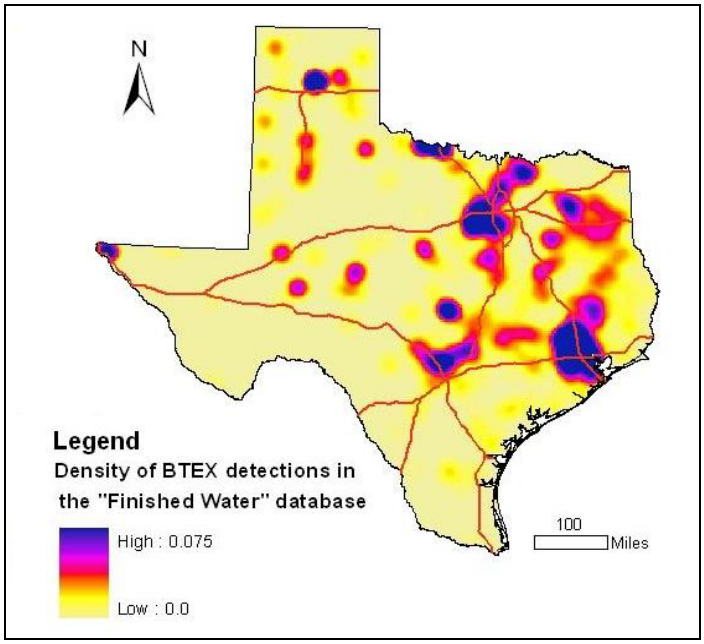

Figure 22 - Density of BTEX detections in the “Finished Water” database

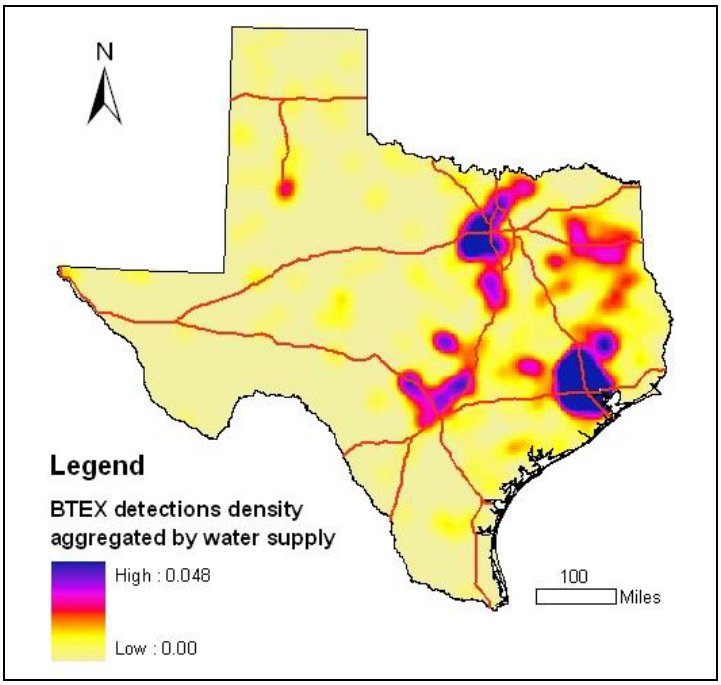

Figure 23 - Density of BTEX detections aggregated by water supply

The above maps demonstrate the differences between the methods of aggregation. Although the spatial distribution is similar in both cases the density of detections varies considerably when different aggregations are used. This can be explained by the assignment of contaminants to a number of wells contributing to a monitoring point in the "Finished Water" database. When aggregating by water supply only one detection is considered.

The following example illustrates a case where the densities computed are considerably different depending on the aggregation method. The first map shows an area of high density when the "Finished Water" database is used and the second map shows the same area when the results are aggregated by water supply.

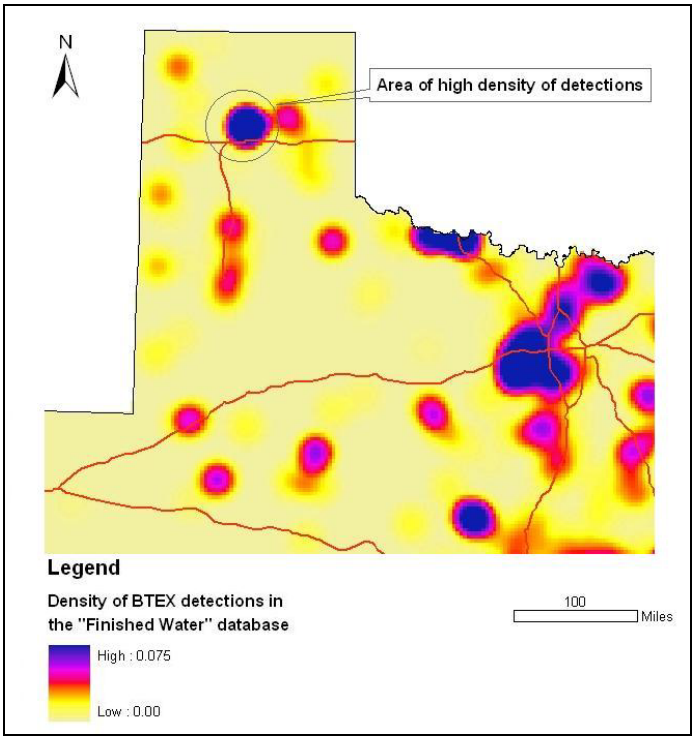

Figure 24 - High density of BTEX detections in the “Finished Water” database

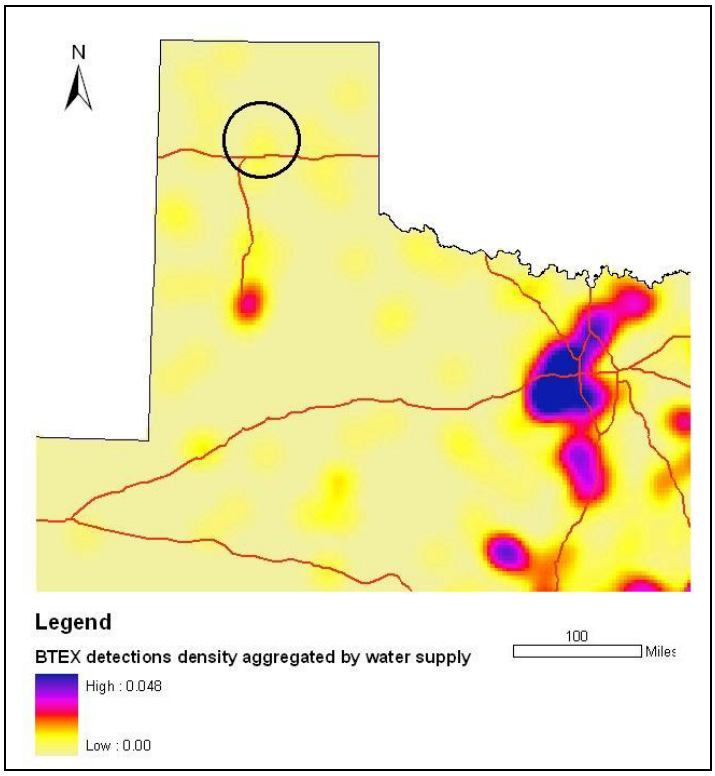

Figure 25 - Density of BTEX detections when aggregated by PWS

The comparison of figures 24 and 25 shows a large variation between the aggregation methods.

A closer look at the detection points created by the different methods may explain the difference in densities shown in the above maps. The following map shows detections of BTEX using both methods. The bright red points are wells treated as contaminated in the "Finished Water" database while the darker point is the well selected to represent the water supply in the aggregated dataset. This example explains the differences in the density maps between the two methods. Although the spatial distribution of the detections is the same, aggregating the detections by water supply will result in lower densities in some cases.

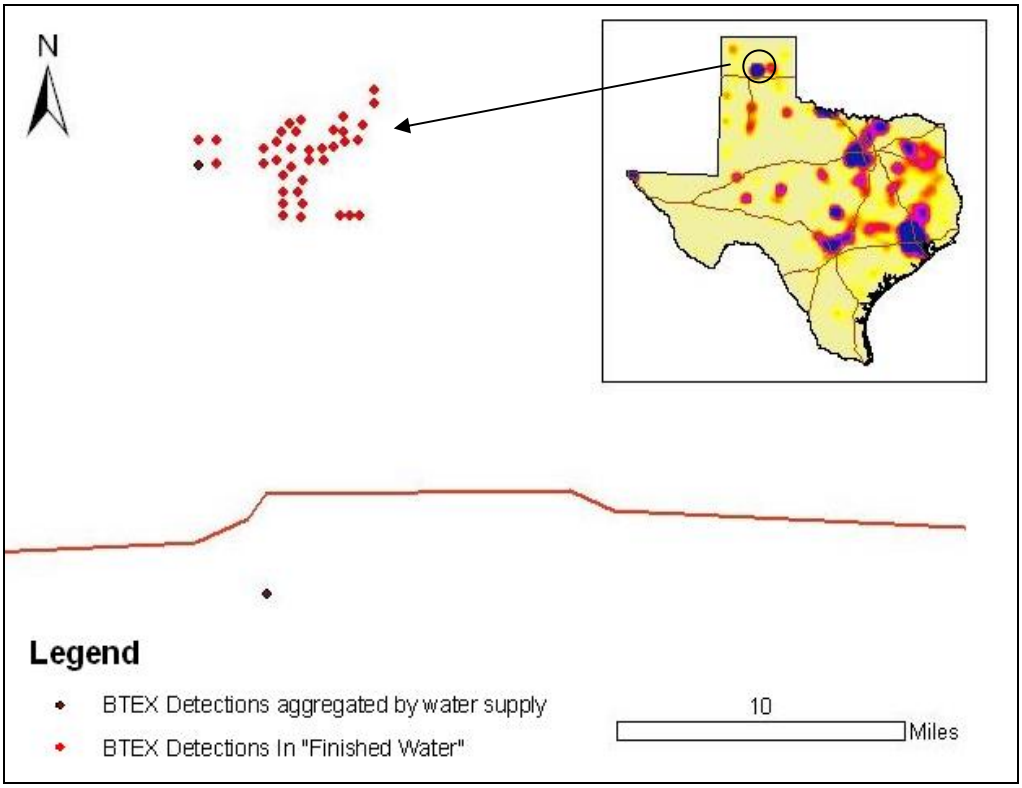

Figure 26 - BTEX detections for both methods of aggregation

4.2.3 SPATIAL DISTRIBUTION OF THE DILUTION ATTENUATION RESULTS

The dilution attenuation component results in a conservative estimation of the concentrations reaching a well from a specific contamination source. A number of aggregation schemes can be used to combine the individual influences of the sources of contamination into one overall concentration for the well. The source water assessment program uses the average concentration in the process of determining susceptibility. Therefore the average concentration is used to aggregate the individual results from the dilution attenuation component and compare these results with the water quality detections.

The results of the dilution attenuation calculation were classified into three categories: high, medium and low. These groupings were established by comparing the average concentration computed for the well with the water quality thresholds and standards described in table 10. Concentrations lower than the threshold were considered as low, between the threshold and half the water quality standard were considered medium and the concentrations exceeding half the water quality standard were assigned to the high category.

Figures 27 and 28 show the wells for which high concentrations of BTEX and TCE group compounds were computed.

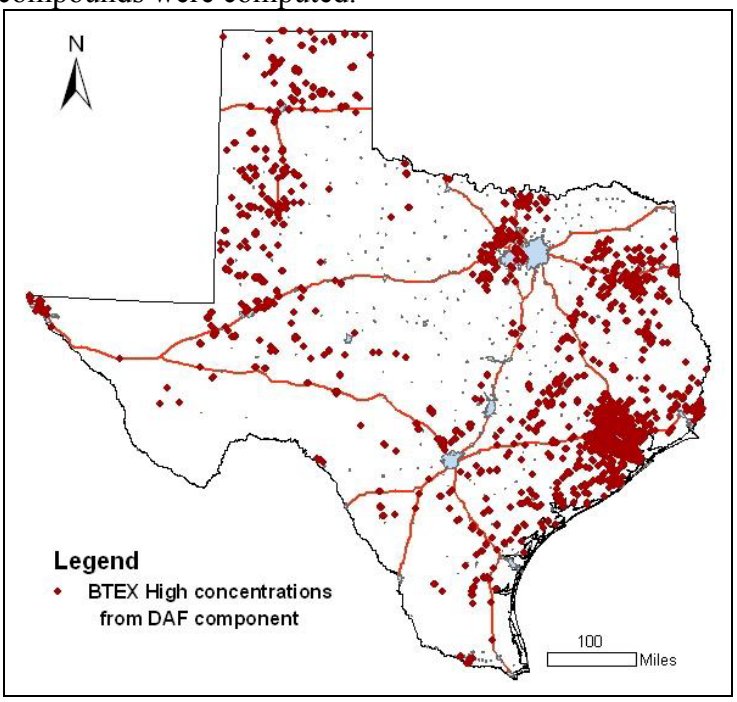

Figure 27 - High BTEX concentrations computed in the dilution attenuation component

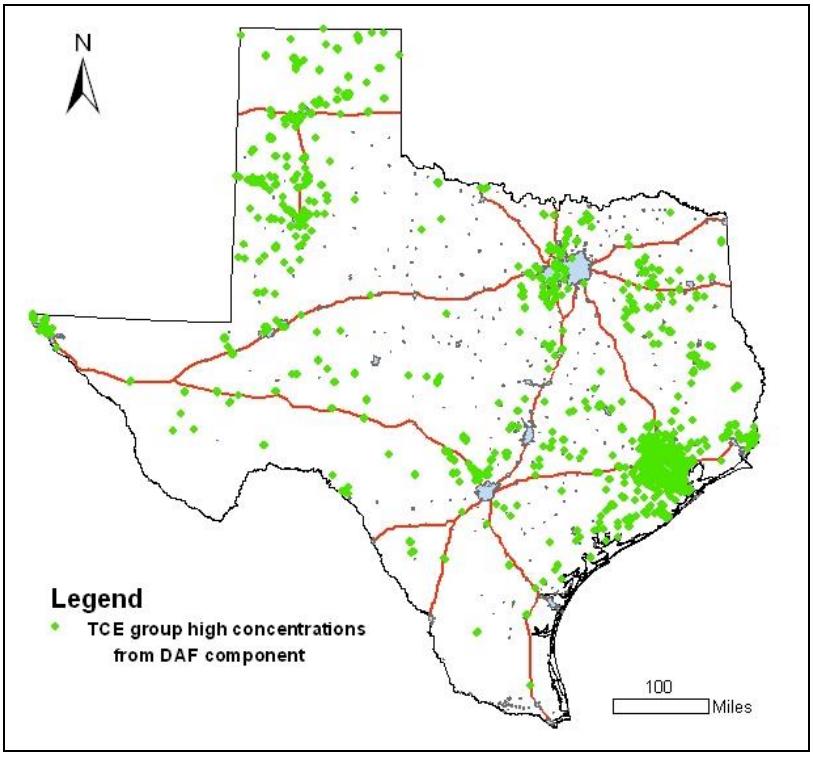

Figure 28 - TCE (and TCE products) High concentrations computed in the dilution attenuation component

Results of the dilution attenuation component were converted into density maps and the water quality detections were compared with these density maps to assess the correlation between the high concentration category of the dilution attenuation results and the water quality detections. The following maps show the relationship between the water quality detections and the dilution attenuation component results for BTEX and TCE group compounds.

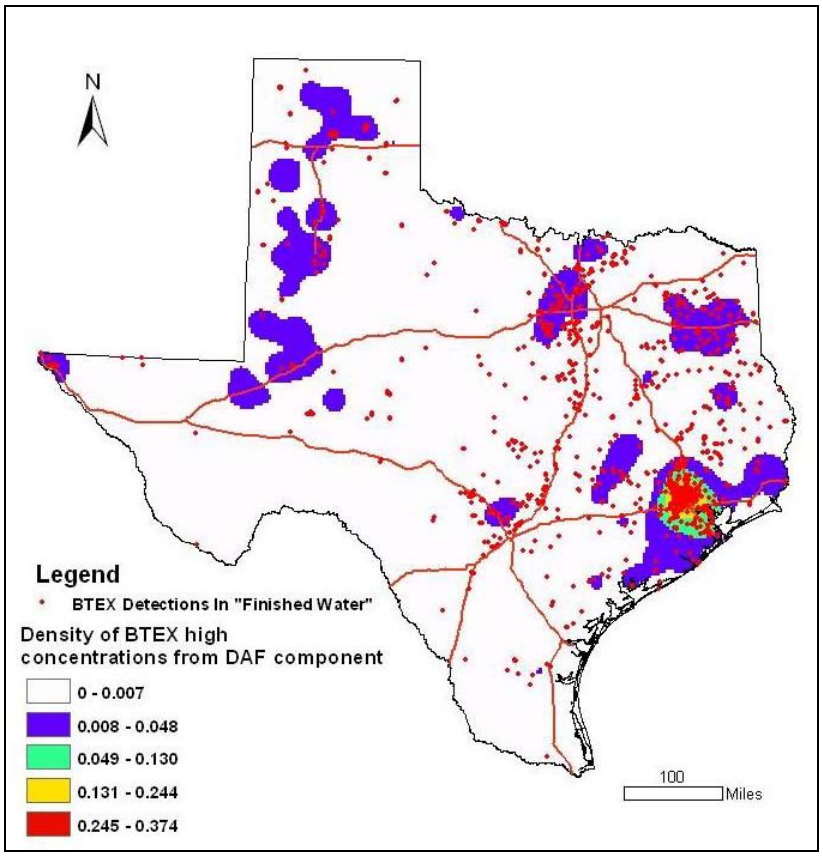

Figure 29 - BTEX detections in the "Finished Water" database overlying a density map of high concentrations from the dilution attenuation component

The above map shows the relationship between the density of high concentrations, from the dilution attenuation component, and the detections of BTEX in the "Finished Water" database. This correlation is especially strong in the denser areas while in the less dense areas the relationship is weaker.

Figure 30 presents the same concept for the TCE group compounds (TCE and TCE degradation products), the map also shows correlation in the denser

areas, where more high concentrations were predicted with the dilution attenuation model.

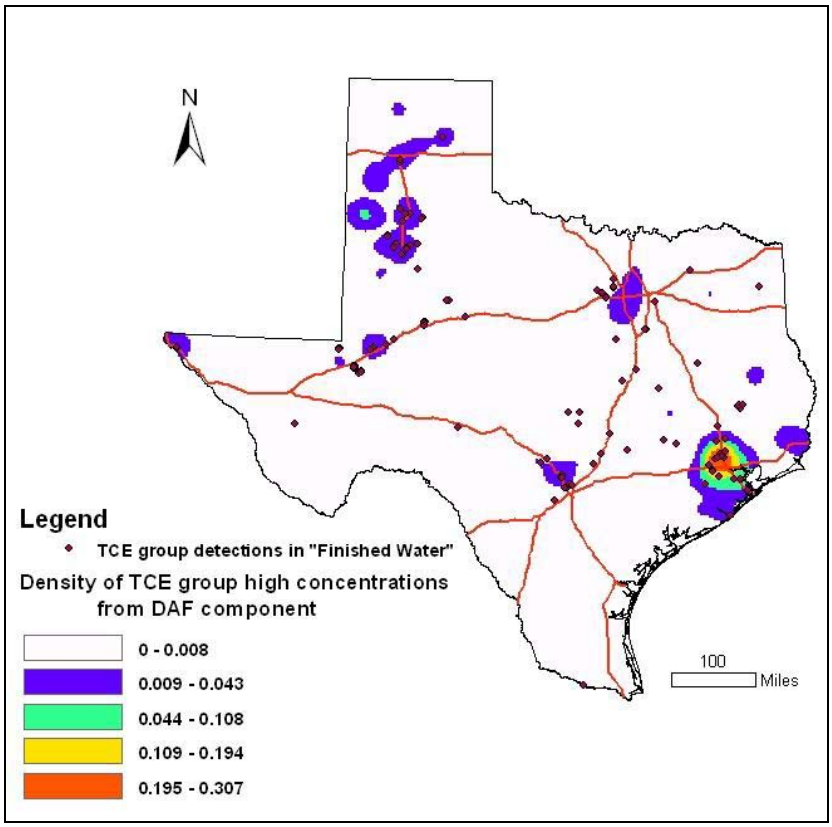

Figure 30 - TCE group detections in the "Finished Water" overlying a density map of high concentrations from the dilution attenuation component

In both of the above maps there are areas with elevated densities of high concentrations from the dilution attenuation model but few detections shown in the water quality database. The dilution attenuation model is conservative and the concentrations estimated with the model should yield higher and more frequent concentrations then the ones actually monitored. This may result in areas where

the model predicts high concentrations but the water quality measurements don't show elevated concentrations.

The following figures show the density of the dilution attenuation component high predictions for BTEX and TCE compounds, compared with the density of detections in the "Finished Water database". The figures on the left show the detections density and the right figures present the densities of the predicted high concentrations.

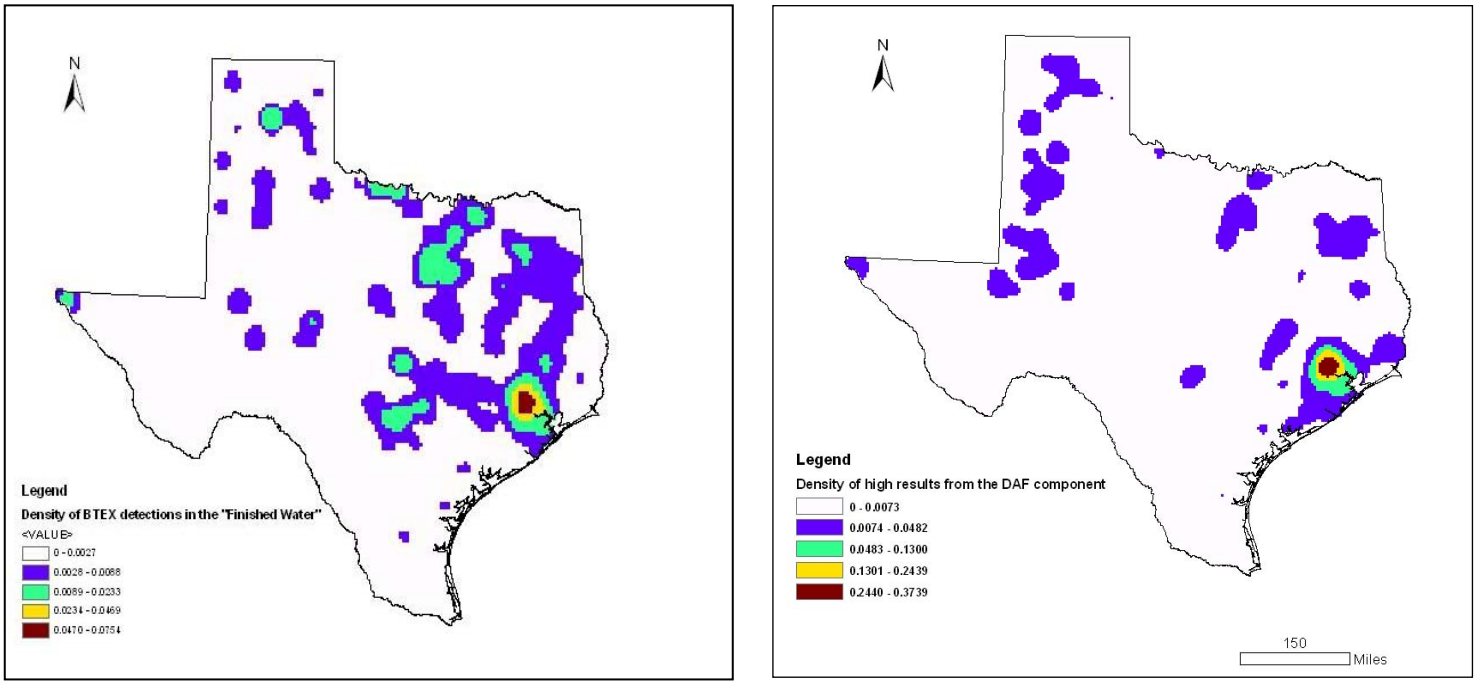

Figure 31 - Densities of monitored (left) and predicted (right) high concentrations for BTEX compounds

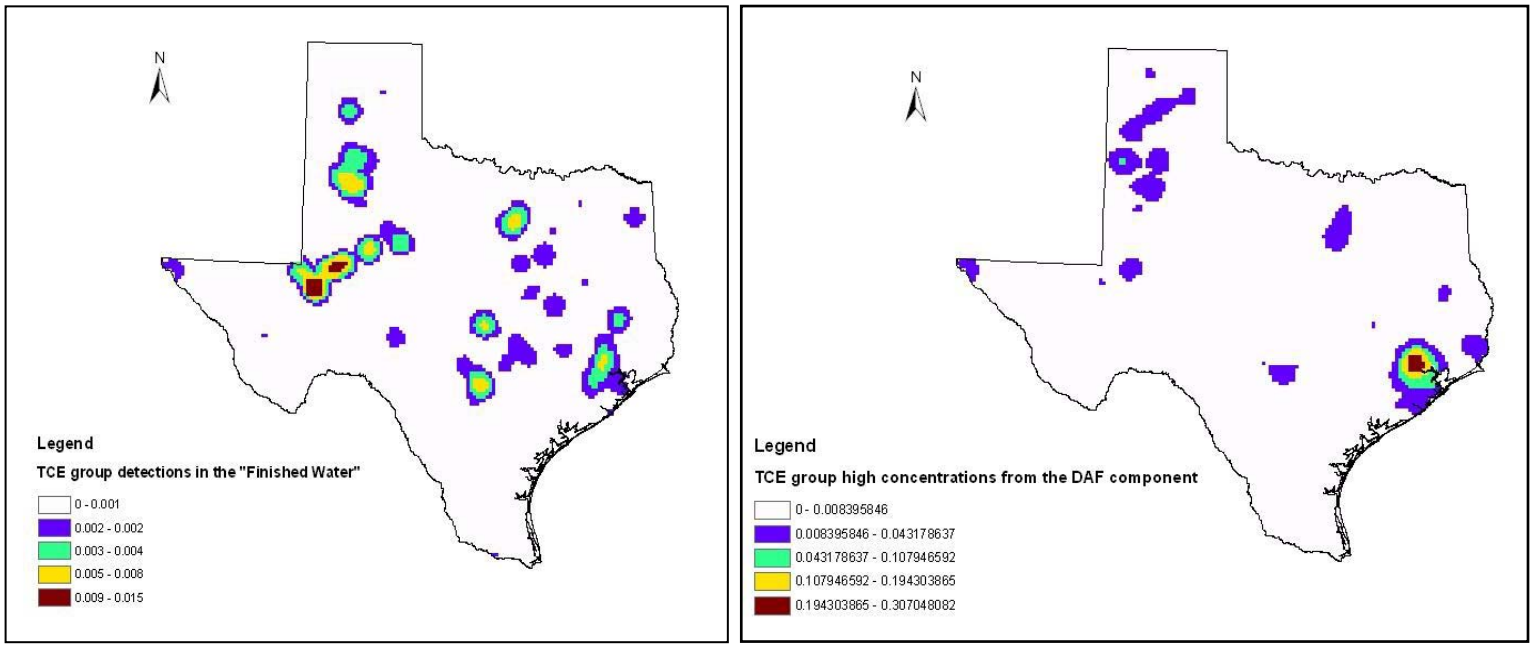

Figure 32 - Densities of monitored (left) and predicted (right) high concentrations for TCE group compounds

Figures 31 and 32 demonstrate the variations between the predicted results and the monitored results. Although some areas with high density of monitoring detections can be predicted with the model, many still are not predicted accurately. This highlights the difficulty in modeling areas of high susceptibility on such a large scale, with variations in aquifer and soil properties.

4.2.4 INFLUENCE OF AQUIFER PROPERTIES

The influence of aquifer properties on the susceptibility of water supplies is examined through two case studies. The Houston and Dallas metropolitan areas were selected as sample study areas. Both areas have high densities of contaminant sources and wells (see figures 15, 16 and 18) but the aquifers from which water is derived have considerably varying properties. Houston area wells are mostly screened in the coastal lowlands aquifer system, especially in the Chicot and Evangeline aquifers. The wells in the Dallas area discharge from the Trinity aquifer system in particular from the Faluxy and Travis Peak formations.

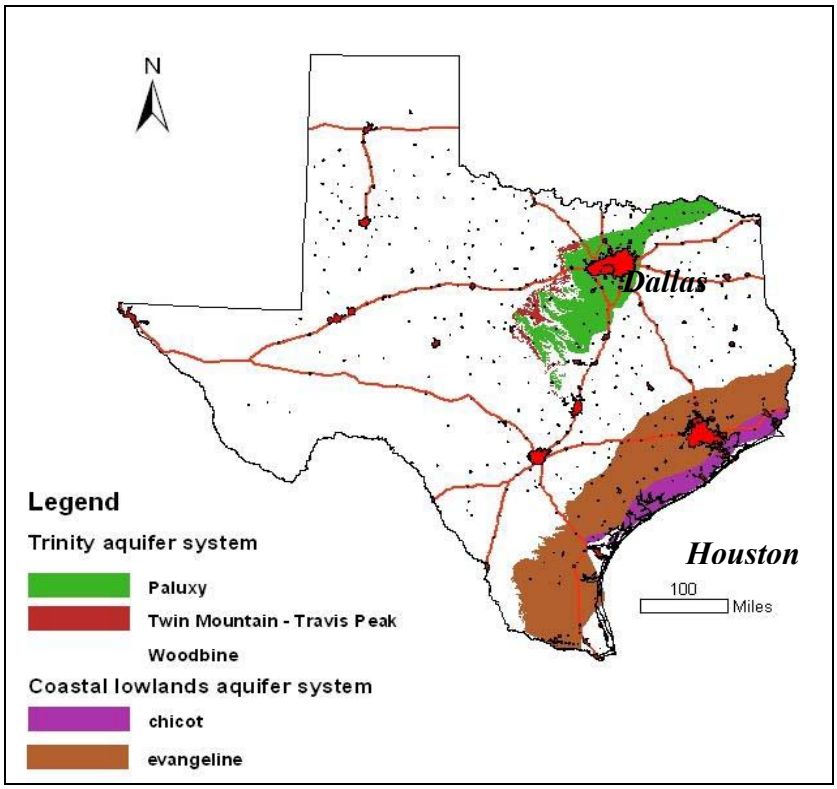

Figure 33 - Trinity and Coastal lowlands aquifer systems

The lithology of the Coastal lowland aquifer system, also known as the "Gulf Coast aquifer" is generally sand, silt and clay. The Chicot and Evangeline aquifers are hydrogeologic designations for subdivisions of the upper mostly sandy part of the system (USGS, 1996). The Chicot aquifer is the top part of the formation and is unconfined in the Houston area. The Evangeline aquifer underlies the Chicot aquifer and is a confined aquifer. These formations are shown in the following diagram from the USGS ground water atlas (USGS, 1996).

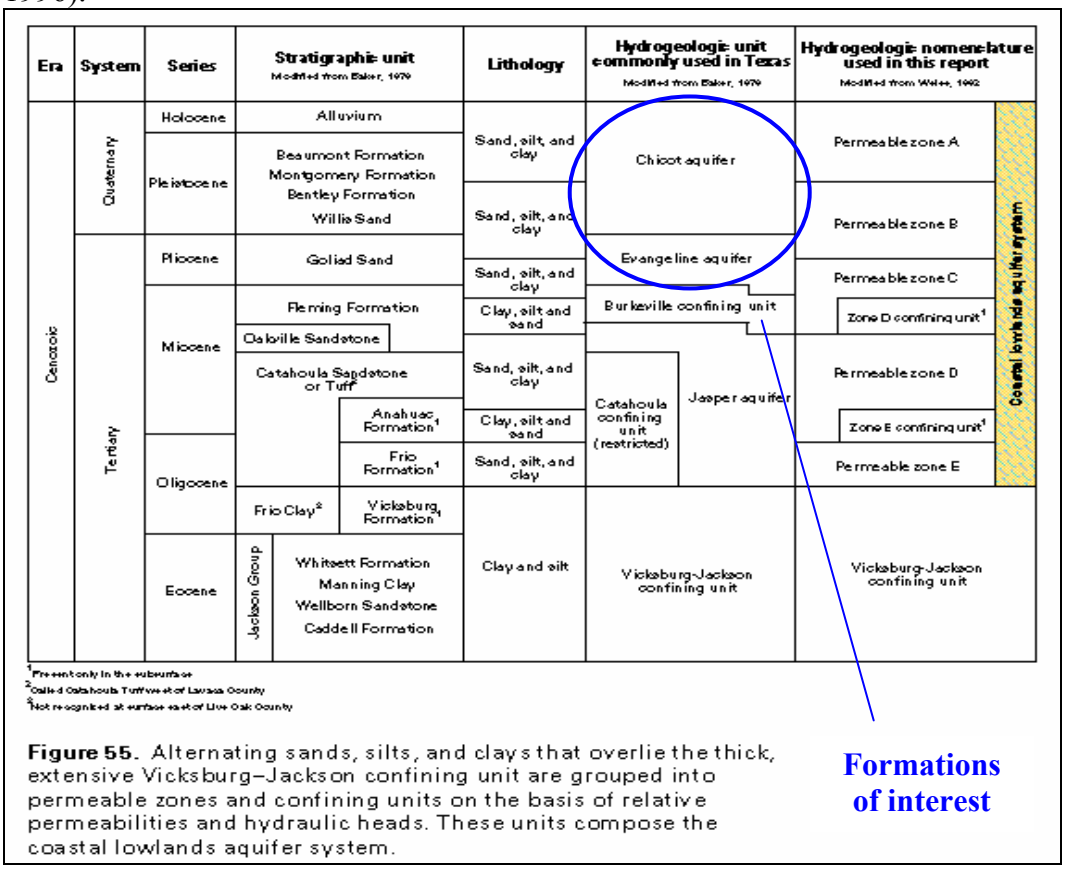

Figure 55. Alternating sands, silts, and clays that overlie the thick, extensive Vicksburg–Jackson confining unit are grouped into permeable zones and confining units on the basis of relative permeabilities and hydraulic heads. These units compose the coastal lowlands aquifer system.

Figure 34 - Correlation chart of the coastal lowlands aquifer system (USGS, 1996)

The Trinity aquifer in its east central and northeastern areas consists of the Twin Mountains, Glen Rose and Paluxy formations (USGS, 1996). The Walnut formation confines the aquifer in these areas. The arrangement of these formations is illustrated in the following diagram together with the formations of the Edwards aquifer.

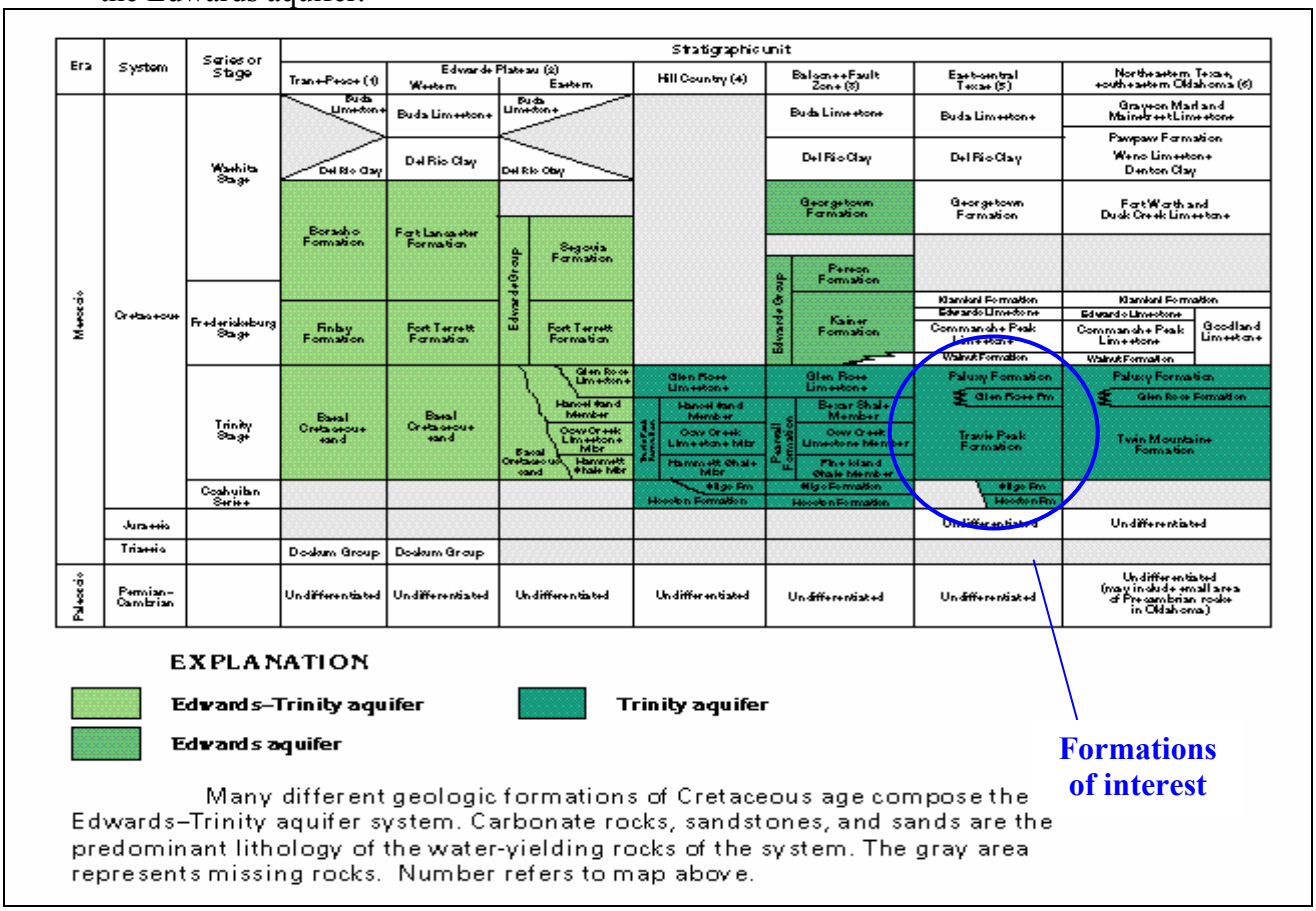

Figure 35 - Correlation chart of the Edwards - Trinity aquifer system (USGS, 1996)

The above correlation diagrams illustrate the difference between the aquifer systems. Wells in the Houston area are screened mostly in the upper sandy

formations. These aquifers should be more susceptible to contamination because of the short distance between the surface and the aquifer and the lack of a thick confining unit. Wells in the Dallas area are mostly screened in deeper formations (Faluxy and Travis Peak), which are overlaid by a confining unit (Walnut formation). The increased distance between the surface and the presence of a confining formation should result in less susceptibility to contamination.

The influence of the varying aquifer systems is analyzed by comparing the water quality detections in both areas. A density map of BTEX and TCE group contaminants detections was produced to compare the number of detections per area in both study cases. A closer look at the study area reveals differences in the patterns of detections.

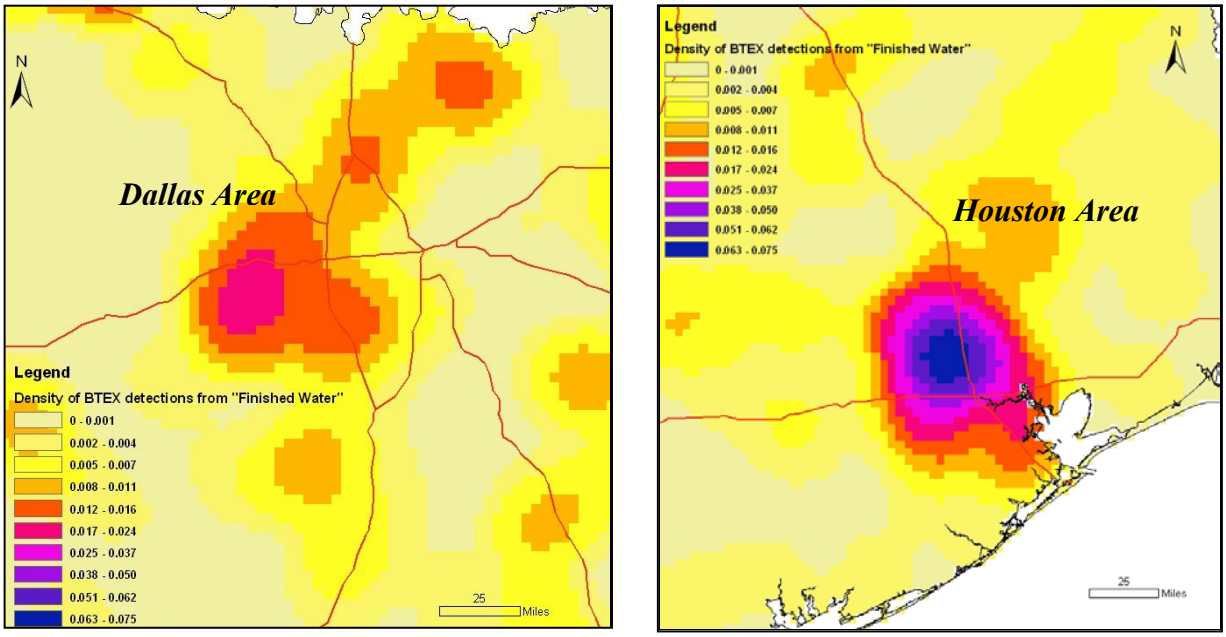

Figure 36 - Density of BTEX detections in the Dallas and Houston areas

Figure 36 shows the difference in the density of BTEX detections from the "Finished Water" database. The map shows that the Houston area has higher

densities of BTEX detections than the Dallas area. This difference may be related to the different aquifer systems, where the unconfined upper aquifers (Chicot and Evangeline), in the Houston area, exhibit more detections per square kilometer than the deeper and confined aquifer (Faluxy and Travis Peak), in the Dallas area. Although this relationship is reasonable, this variability can also be related to variations in the sources of contamination densities and the spatial distribution of the wells. A similar analysis was performed for TCE and its degradation products (referred to as TCE group), and the results are shown in Figures 37 - 39.

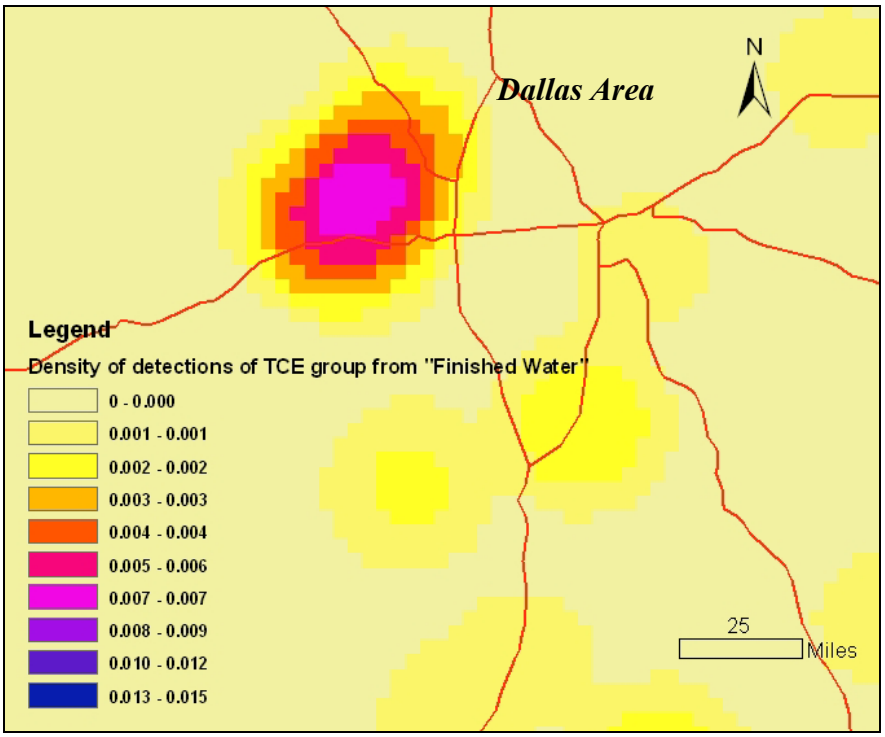

Figure 37 - Density of detections of TCE group contaminants in the Dallas area from the “Finished Water” database

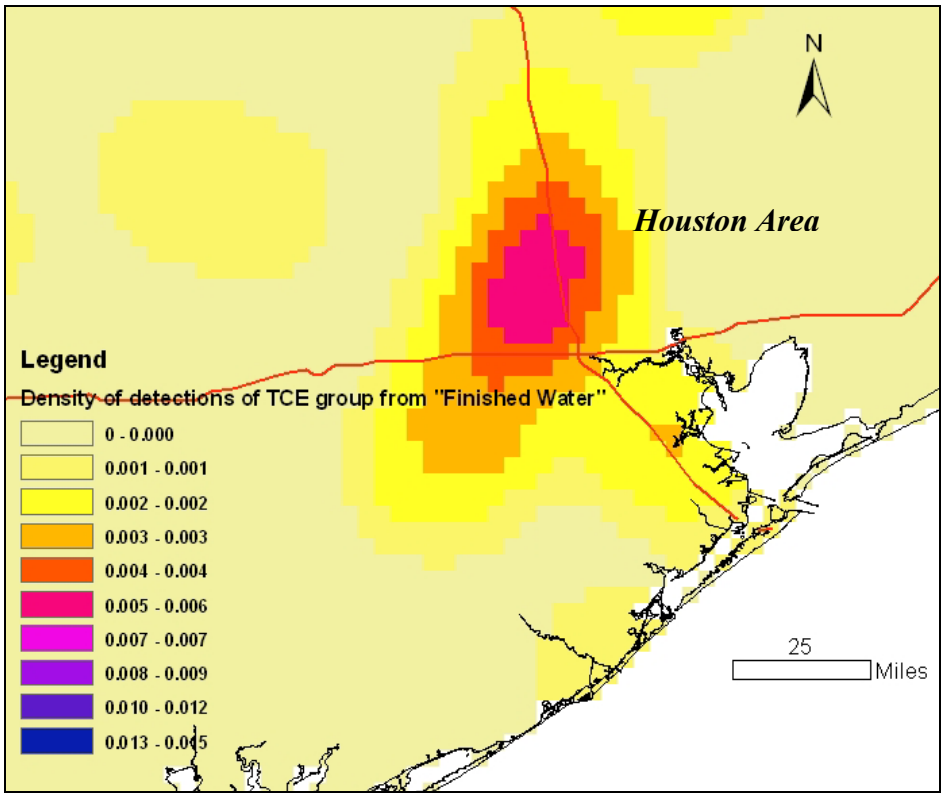

Figure 38 - Density of detections of TCE group contaminants in the Houston area from the "Finished Water" database

The density of TCE detections near the Dallas area is higher than the one in the Houston area. This result contradicts the assumption that wells in the Houston area are more susceptible to contamination than in the Dallas area. This contradiction may be related to the small number of detections in the "Finished Water" dataset. Due to the small number of detections, the spatial patterns are hard to distinguish and high density spots may be created from superficial patterns in the database. These unrealistic local patterns may occur when a number of

wells are treated as contaminated because they are related to one monitoring point. To eliminate these trends the detections were aggregated by water supply.

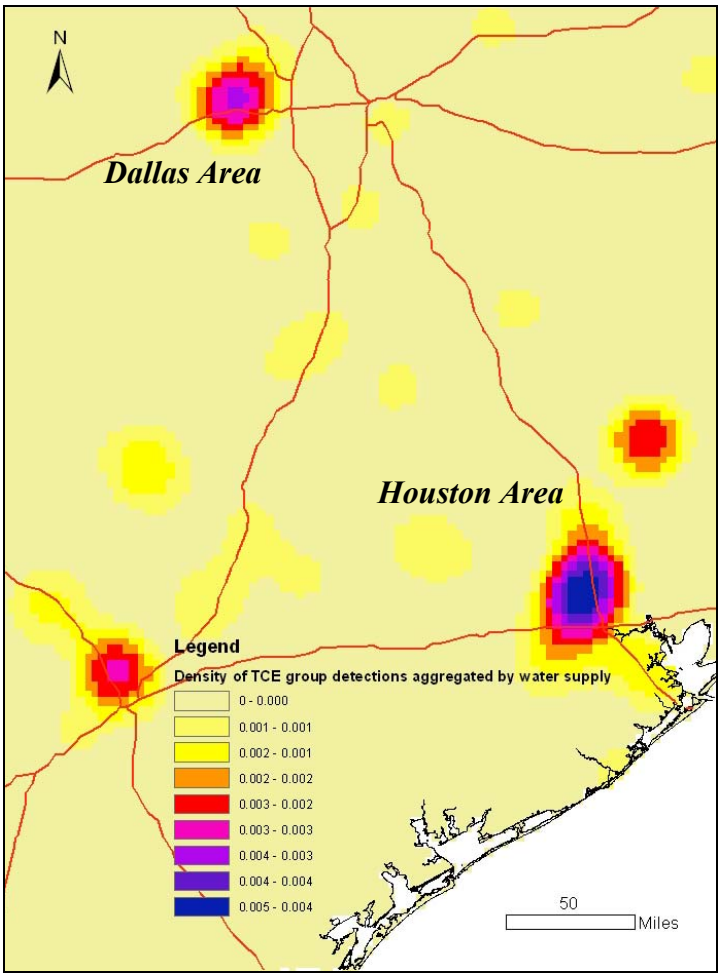

Figure 39 - Density of detections of TCE group contaminants from the aggregated "Finished Water" database

Figure 39 shows that when aggregating the TCE results by water supply the spatial trends are considerably different than the trends observed without the aggregation. When the aggregated dataset is used to compute the density of

detections the Houston area has higher densities than the Dallas area. This distribution is more reasonable when considering the aquifer systems.

The above results demonstrate the importance of the aggregation methods on the spatial trends of detections. These trends can be analyzed to determine more susceptible areas and to find relationships between the aquifers characteristics and the susceptibility of wells to contamination.

5. CONCLUSIONS

Determining the susceptibility of water supplies to contamination is a complex problem, which involves identification of sources of contamination and assessing the effects these sources might have on water quality. To understand the relationship between the sources of contamination and the water supply wells one must model the transport of contaminants from the point of introduction to the environment through the subsurface to the assessed well.

The tier 2 model applied in the Texas source water assessment program gives a physical relationship between point sources of contamination and water supply wells. The model describes the dilution and attenuation of contaminants in the groundwater transport using well-established leaching and transport formulations. The focus of this study is to establish a model that provides a numerical link between potential sources of contamination and water supply wells. The model includes the major natural processes taking place in the environment during contaminants migration in groundwater systems. These processes include dilution, sorption, dispersion and degradation. This numerical connection enables the calculation of expected contaminant concentrations and these can be used to better estimate the susceptibility of water supplies to contamination.

The model proposed is executable on a large scale, due to extensive dataset construction under the Texas source water assessment program by the USGS and TCEQ and the capabilities introduced through GIS software. The detailed information developed in the program enables the use of a screening model (tier 2), which requires site specific properties of aquifers and soils, on a regional scale.

Another important aspect of the study is the construction of the chemical database containing physical-chemical properties and degradation rates, necessary to model the variety of contaminants and their behavior in the environment. The chemical database includes conservative estimates of chemical properties that effect the concentration reduction during the transport in groundwater systems. These parameters have a large impact on the models results and in some cases dominate the contaminants interaction within the environment. The variability in these parameters is large, thus making it difficult to select one representative value to model the contaminant. This is particularly true for metals for which interactions are dependent on a variety of factors such as pH, water composition and precipitation of solids. Future studies should address these issues once the initial assessments are analyzed. More detailed representation of the chemical properties might be necessary to model certain contaminants, perhaps by using aquifer specific water compositions and pH to model the contaminants interactions within the aquifers. This is especially important in the estimation of solubility values of metals, which are used to determine the initial concentration

at the source of contamination. A different approach, such as using observed concentrations as the source concentration, may be more suitable.

Comparison of the results from the dilution attenuation component with water quality detections did not show high correlation. Only up to 38% of the public water supplies with water quality detections had identified sources of contamination, resulting in low prediction rates of the model. It appears that many detections are present where no sources of contamination are identified, suggesting the need for better identification of contamination sources to better predict the susceptibility from point sources.

The magnitude of the task undertaken has effect on the models precision. Accurately assessing more than 13,000 wells, over the entire state of Texas, with varying aquifers and soil properties is a challenging task. Although the accuracy rates of the model appear to be low, it is important to keep in mind that this component is only one of a number of methods used to determine susceptibility. These include susceptibility from non point sources, intrinsic susceptibility and contaminant occurrences. When combined together these should yield a more accurate analysis of the susceptibility.

The use of spatial functions in ArcGIS shows promising prospects in susceptibility studies. The examples shown highlight the importance of the spatial patterns and how they might relate to water quality. Interpolation of properties such as the density of contaminant sources and wells can help in determining areas of higher susceptibility. The results presented are initial results from the Texas source water assessment program. USGS and TCEQ are undergoing a

process of executing the susceptibility assessment and verifying the results. More detailed studies of the models results and the correlation of contaminant occurrence, well density and aquifer properties are recommended to better understand these patterns and relationships.

Finally, this method will hopefully contribute to the development of better susceptibility assessments by incorporating site-specific models (such as the tier 2 model) into regional assessments. The execution of these models permits a more accurate and detailed description of contaminants introduced into the environment and their transport and interaction within groundwater systems.

APPENDIX 1 – LIST OF CONTAMINANTS WITH CHEMICAL PHYSICAL PROPERTIES

The following table shows the final list of contaminants and their physical-chemical properties. These properties were used in the Tier 2 model to calculate the dilution attenuation factor. A full description of the database development, the assumptions and sources of information used in its construction are given in section 3.5.2.

Description of the fields

- CD – Identifier number of the contaminant used in the Texas Source Water Assessment Program
- CAS – CAS number in the TRRP PCL table.
- CONTAMINANT – Name of the contaminant
- TYPE – the type of the contaminant, organic (O), inorganic (I) or metal (M).
- H – Selected Henry's law constant (dimensionless).
- LOG KOC – The log of selected Koc values (cm^3-water/g-carbon).
- SOLUBILITY - Selected solubility value (mg/l).

CD	CAS	CONTAMINANT	TYPE	H	LogKd	LOGKOC	SOLUBILITY	Dg
1	630-20-6	1,1,1,2-TETRACHLOROETHANE	O	9.977E-02	none	2.543	1.100E+03	1.801E-05
2	71-55-6	1,1,1-TRICHLOROETHANE	O	7.116E-01	none	2.040	1.330E+03	2.204E-06
3	79-34-5	1,1,2,2-TETRACHLOROETHANE	O	1.518E-02	none	1.890	2.970E+03	2.735E-05
4	79-00-5	1,1,2-TRICHLOROETHANE	O	3.409E-02	none	1.502	4.420E+03	1.648E-06
5	75-34-3	1,1-DICHLOROETHANE	O	2.325E-01	none	1.403	5.500E+03	3.343E-06
6	75-35-4	1,1-DICHLOROETHYLENE	O	1.056E+00	none	1.743	2.400E+03	9.117E-06
7	563-58-6	1,1-DICHLOROPROPENE	O	1.819E+00	none	2.143	7.488E+02	6.418E-05
8	87-61-6	1,2,3-TRICHLOROBENZENE	O	3.800E-02	none	3.663	1.884E+01	4.011E-05

CD	CAS	CONTAMINANT	TYPE	H	LogKd	LOGKOC	SOLUBILITY	Dg
9	96-18-4	1,2,3-TRICHLOROPROPANE	O	1.419E-02	none	1.883	1.900E+03	1.671E-06
10	120-82-1	1,2,4-TRICHLOROBENZENE	O	5.874E-02	none	3.220	4.880E+01	3.343E-06
11	95-63-6	1,2,4-TRIMETHYLBENZENE	O	1.840E-01	none	2.970	7.959E+01	2.149E-05
12	107-06-2	1,2-DICHLOROETHANE	O	4.882E-02	none	1.093	8.700E+03	3.343E-06
13	78-87-5	1,2-DICHLOROPROPANE	O	1.168E-01	none	1.593	2.800E+03	4.668E-07
14	122-66-7	1,2-DIPHENYLHYDRAZINE	O	1.422E-07	none	2.553	1.840E+03	3.343E-06
15	108-67-8	1,3,5-TRIMETHYLBENZENE	O	2.720E-01	none	3.010	5.148E+01	6.418E-05
16	541-73-1	1,3-DICHLOROBENZENE	O	1.088E-01	none	2.230	1.100E+02	3.343E-06
17	142-28-9	1,3-DICHLOROPROPANE	O	4.038E-02	none	1.613	2.157E+03	6.418E-05
18	542-75-6	1,3-DICHLOROPROPENE	O	1.226E-01	none	1.642	1.994E+03	6.418E-05
19	594-20-7	2,2-DICHLOROPROPANE	O	3.394E-01	none	2.192	1.682E+03	6.418E-05
20	1746-01-6	2,3,7,8-TCDD	O	1.474E-03	none	6.413	1.103E-03	1.020E-06
21	93-76-5	2,4,5-T	O	2.826E-07	none	2.474	2.780E+02	6.685E-06
22	93-72-1	2,4,5-TP	O	3.748E-07	none	3.413	1.400E+02	6.418E-05
23	88-06-2	2,4,6-TRICHLOROPHENOL	O	1.076E-04	none	2.117	9.820E+02	6.610E-07
24	94-75-7	2,4-D	O	5.820E-09	none	2.423	8.900E+02	6.685E-06
25	120-83-2	2,4-DICHLOROPHENOL	O	9.060E-05	none	1.857	4.500E+03	2.799E-05
26	51-28-5	2,4-DINITROPHENOL	O	2.012E-07	none	-2.000	5.800E+03	2.288E-06
27	121-14-2	2,4-DINITROTOLUENE	O	2.234E-06	none	1.593	4.462E+02	3.343E-06
28	606-20-2	2,6-DINITROTOLUENE	O	3.090E-05	none	1.620	3.524E+02	3.343E-06
29	95-49-8	2-CHLOROTOLUENE	O	1.347E-01	none	2.610	1.540E+02	6.418E-05
30	591-78-6	2-HEXANONE	O	3.381E-03	none	0.993	1.794E+04	2.777E-04
31	95-48-7	2-METHYLPHENOL	O	4.964E-05	none	1.562	2.040E+04	8.596E-05
32	16655-82-6	3-HYDROXYCARBOFURAN	O	2.466E-12	none	0.373	6.207E+03	6.418E-05
33	106-43-4	4-CHLOROTOLUENE	O	1.335E-01	none	2.696	1.358E+02	6.418E-05
34	99-87-6	4-ISOPROPYLTOLUENE	O	4.551E-01	none	3.360	2.788E+01	1.605E-04
35	108-10-1	4-METHYL-2-PENTANONE	O	5.709E-03	none	0.923	1.900E+04	8.596E-05
36	83-32-9	ACENAPHTHENE	O	6.443E-03	none	3.533	4.240E+00	5.899E-06
37	208-96-8	ACENAPHTHYLENE	O	4.739E-03	none	3.553	3.930E+00	1.003E-05
38	34256-82-1	ACETOCHLOR	O	9.225E-07	none	2.642	2.230E+02	4.011E-05
39	67-64-1	ACETONE	O	1.613E-03	none	-0.627	6.000E+05	8.596E-05
40	107-13-1	ACRYLONITRILE	O	5.709E-03	none	-0.137	7.500E+04	2.616E-05
41	15972-60-8	ALACHLOR	O	3.442E-07	none	2.279	2.400E+02	4.011E-05
42	116-06-3	ALDICARB	O	5.820E-08	none	0.743	6.000E+03	1.895E-06
43	1646-88-4	ALDICARB SULFONE	O	1.096E-07	none	-0.959	8.000E+03	6.418E-05
44	1646-87-3	ALDICARB SULFOXIDE	O	4.009E-08	none	-1.167	2.800E+04	6.418E-05
45	309-00-2	ALDRIN	O	1.820E-03	none	4.680	7.840E-02	1.017E-06
47	14903-36-7	Aluminum Cation	M	0.000E+00	4.914E-01	none	1.148E+00	0.000E+00
48	120-12-7	ANTHRACENE	O	2.300E-03	none	4.064	6.905E-01	1.308E-06

CD	CAS	CONTAMINANT	TYPE	H	LogKd	LOGKOC	SOLUBILITY	Dg
49	64924-52-3	Antimonate	M	0.000E+00	-1.800E+01	none	NoValueReported	0.000E+00
50	53469-21-9	AROCLOR	O	7.860E-03	none	5.903	2.770E-01	1.605E-05
51	15584-04-0	Arsenate	M	0.000E+00	1.462E+00	none	NoValueReported	0.000E+00
52	1332-21-4	ASBESTOS	I	0.000E+00	-1.800E+01	none	NoValueReported	0.000E+00
53	1912-24-9	ATRAZINE	O	9.763E-08	none	2.204	2.141E+02	4.011E-05
54	16541-35-8	Barium Cation	M	0.000E+00	1.613E+00	none	1.336E+04	0.000E+00
55	25057-89-0	BENTAZON	O	9.019E-08	none	1.953	5.000E+02	6.418E-05
56	71-43-2	BENZENE	O	2.274E-01	none	1.743	2.000E+03	1.671E-06
57	56-55-3	BENZO(A)ANTHRACENE	O	1.393E-04	none	5.373	2.907E-02	8.848E-07
58	50-32-8	BENZO(A)PYRENE	O	1.891E-05	none	5.740	1.038E-02	4.011E-05
59	205-99-2	BENZO(B)FLUORANTHENE	O	2.718E-05	none	5.393	2.065E-02	9.864E-07
60	191-24-2	BENZO(G,H,I)PERYLENE	O	1.369E-05	none	6.200	2.842E-03	9.257E-07
61	207-08-9	BENZO(K)FLUORANTHENE	O	4.448E-07	none	5.723	1.079E-02	2.812E-07
62	14701-08-7	Beryllium ion	M	0.000E+00	2.898E+00	none	1.190E+01	0.000E+00
63	71-52-3	BICARBONATE	I	1.168E+00	-1.800E+01	none	NoValueReported	0.000E+00
64	11113-50-1	Boric acid	I	0.000E+00	-1.800E+01	none	NoValueReported	0.000E+00
65	314-40-9	BROMACIL	O	4.344E-09	none	1.723	8.150E+02	6.418E-05
66	24959-67-9	BROMIDE	I	0.000E+00	-1.800E+01	none	NoValueReported	0.000E+00
67	108-86-1	BROMOBENZENE	O	8.382E-02	none	2.384	4.460E+02	6.418E-05
68	74-97-5	BROMOCHLOROMETHANE	O	3.690E-02	none	1.021	2.042E+04	1.605E-04
69	75-27-4	BROMODICHLOROMETHANE	O	8.770E-02	none	1.613	4.500E+03	6.418E-05
70	75-25-2	BROMOFORM	O	2.213E-02	none	1.940	3.200E+03	3.343E-06
71	74-83-9	BROMOMETHANE	O	2.581E-01	none	0.803	1.520E+04	3.167E-05
72	23184-66-9	BUTACHLOR	O	2.110E-06	none	4.114	2.300E+01	6.418E-05
73	85-68-7	BUTYL BENZYL PHTHALATE	O	5.213E-05	none	4.138	2.900E+00	6.685E-06
74	22537-48-0	Cadmium cation	M	0.000E+00	4.314E-01	none	1.095E+04	0.000E+00
75	14102-48-8	Calcium cation	M	0.000E+00	0.00	none	3.922E+03	0.000E+00
76	63-25-2	CARBARYL	O	1.804E-07	none	1.973	4.162E+02	2.006E-05
77	1563-66-2	CARBOFURAN	O	1.278E-07	none	1.462	7.000E+02	6.418E-05
78	75-15-0	CARBON DISULFIDE	O	5.957E-01	none	1.553	2.928E+03	1.605E-04
79	56-23-5	CARBON TETRACHLORIDE	O	1.142E+00	none	2.270	8.050E+02	3.343E-06
80	3812-32-6	CARBONATE	I	1.179E+03	-1.800E+01	none	NoValueReported	0.000E+00
81	57-74-9	CHLORDANE	O	2.011E-03	none	5.080	5.600E-02	4.341E-07
82	5103-71-9	CHLORDANE (ALPHA-CHLORDANE)	O	2.011E-03	none	5.833	4.640E-02	1.605E-05
83	12789-03-6	CHLORDANE (GAMMA-CHLORDANE)	O	2.011E-03	none	5.833	1.299E-02	1.605E-05
84	39765-80-5	CHLORDANE (TRANS-NONACHLOR)	O	1.026E-03	none	5.963	6.120E-03	1.605E-05
85	16887-00-6	CHLORIDE	I	0.000E+00	-1.800E+01	none	NoValueReported	0.000E+00
86	108-90-7	CHLOROBENZENE	O	1.287E-01	none	2.330	5.020E+02	4.011E-06
87	75-00-3	CHLOROETHANE	O	2.120E-01	none	1.041	2.000E+04	2.149E-05
88	67-66-3	CHLOROFORM	O	1.518E-01	none	1.583	7.920E+03	6.685E-07

CD	CAS	CONTAMINANT	TYPE	H	LogKd	LOGKOC	SOLUBILITY	Dg
89	74-87-3	CHLOROMETHANE	O	3.649E-01	none	0.522	2.262E+04	2.149E-05
90	17493-86-6	Chromate	M	0.000E+00	1.279E+00	none	1.274E-02	0.000E+00
91	218-01-9	CHRYSENE	O	5.030E-05	none	5.423	2.635E-02	6.017E-07
92	156-59-2	CIS-1,2-DICHLOROETHYLENE	O	1.688E-01	none	1.462	6.410E+03	6.418E-05
93	10061-01-5	CIS-1,3-DICHLOROPROPENE	O	9.150E-02	none	1.642	2.700E+03	6.418E-05
94	17493-86-6	Copper ion	M	0.000E+00	7.782E-01	none	1.029E+01	0.000E+00
96	21725-46-2	CYANAZINE	O	1.225E-10	none	1.692	1.838E+02	1.605E-05
97	57-12-5	CYANIDE	I	3.406E-03	-1.800E+01	none	NoValueReported	0.000E+00
98	75-99-0	DALAPON	O	3.732E-06	none	1.292	5.020E+05	1.003E-05
99	2136-79-0	DCPA DI-ACID DEGRADATE	O	8.398E-12	none	1.743	1.754E+02	4.011E-05
100	887-54-7	DCPA MONO-ACID DEGRADATE	O	3.351E-09	none	2.803	1.826E+01	4.011E-05
101	72-55-9	DDE	O	8.730E-04	none	5.040	6.500E-02	1.070E-07
102	103-23-1	DI-(2-ETHYLHEXYL)ADIPATE	O	1.795E-05	none	5.580	7.800E-01	2.149E-05
103	117-81-7	DI-(2-ETHYLHEXYL)PHTHALATE	O	1.117E-05	none	7.212	3.000E-01	3.094E-06
104	333-41-5	DIAZINON	O	4.675E-06	none	2.120	4.000E+01	6.418E-05
105	53-70-3	DIBENZ(A,H)ANTHRACENE	O	4.656E-07	none	6.152	3.304E-03	6.401E-07
106	124-48-1	DIBROMOCHLOROMETHANE	O	3.239E-02	none	1.770	5.250E+03	6.685E-06
107	67708-83-2	DIBROMOCHLOROPROPANE	O	6.081E-03	none	2.230	1.000E+03	6.418E-05
108	74-95-3	DIBROMOMETHANE	O	3.401E-02	none	1.312	1.100E+04	2.149E-05
109	1918-00-9	DICAMBA	O	9.019E-08	none	0.342	8.310E+03	6.418E-05
110	75-71-8	DICHLORODIFLUOROMETHANE	O	1.419E+01	none	1.773	2.800E+02	3.343E-06
111	75-09-2	DICHLOROMETHANE	O	9.104E-02	none	0.863	1.540E+04	2.149E-05
112	60-57-1	DIELDRIN	O	1.110E-04	none	4.330	1.950E-01	5.571E-07
113	84-66-2	DIETHYL PHTHALATE	O	1.871E-05	none	2.033	1.080E+03	1.074E-05
114	131-11-3	DIMETHYL PHTHALATE	O	4.344E-06	none	1.500	4.190E+03	8.596E-05
115	84-74-2	DI-N-BUTYL PHTHALATE	O	5.945E-05	none	4.114	1.120E+01	5.232E-05
116	88-85-7	DINOSEB	O	1.886E-05	none	3.080	5.200E+01	4.892E-06
117	2764-72-9	DIQUAT	O	2.690E-12	none	1.973	7.000E+01	1.605E-04
118	298-04-4	DISULFOTON	O	8.936E-05	none	3.632	1.600E+01	2.865E-05
119	330-54-1	DIURON	O	2.085E-08	none	2.292	1.506E+02	6.418E-05
120	145-73-3	ENDOTHALL	O	1.593E-14	none	1.522	1.000E+05	2.777E-04
121	72-20-8	ENDRIN	O	4.947E-05	none	3.970	2.500E-01	1.605E-05
122	759-94-4	EPTC	O	6.578E-04	none	2.823	3.700E+02	6.418E-05
124	97-63-2	ETHYL METHACRYLATE	O	6.651E-03	none	1.553	1.900E+04	1.605E-04
125	100-41-4	ETHYLBENZENE	O	3.260E-01	none	2.310	2.286E+02	5.278E-06
126	106-93-4	ETHYLENE DIBROMIDE	O	2.759E-02	none	1.573	4.320E+03	1.003E-05
128	86-73-7	FLUORENE	O	2.644E-03	none	3.793	1.980E+00	1.003E-05
129	16984-48-8	FLUORIDE	I	0.000E+00	-1.800E+01	none	NoValueReported	0.000E+00
130	944-22-9	FONOFOS	O	2.888E-04	none	3.553	1.070E+01	6.418E-05
132	1071-83-6	GLYPHOSATE	O	1.688E-17	none	-4.387	1.000E+06	1.605E-04

CD	CAS	CONTAMINANT	TYPE	H	LogKd	LOGKOC	SOLUBILITY	Dg
136	76-44-8	HEPTACHLOR	O	1.216E-02	none	4.070	1.800E-01	1.605E-05
137	1024-57-3	HEPTACHLOR EPOXIDE	O	3.446E-04	none	3.859	2.750E-01	1.090E-06
138	118-74-1	HEXACHLOROBENZENE	O	2.224E-02	none	4.450	1.922E-01	2.880E-07
139	87-68-3	HEXACHLOROBUTADIENE	O	4.261E-01	none	3.840	3.200E+00	3.343E-06
140	77-47-4	HEXACHLOROCYCLOPENTADIENE	O	7.150E-01	none	3.980	1.800E+00	1.605E-05
141	15035-72-0	Sulfide	I	4.087E-01	-1.800E+01	none	NoValueReported	0.000E+00
142	193-39-5	INDENO[1,2,3,CD]PYRENE	O	2.852E-06	none	6.312	3.751E-03	8.242E-07
143	74-88-4	IODOMETHANE	O	2.176E-01	none	1.124	1.244E+04	2.149E-05
144	15438-31-0	Iron Ion	M	0.000E+00	4.914E-01	none	1.747E+04	0.000E+00
145	98-82-8	ISOPROPYLBENZENE	O	4.757E-01	none	3.272	7.503E+01	7.521E-05
146	845-52-3	LAMBAST	O	5.171E-11	none	1.963	1.188E+02	4.011E-05
147	14701-27-0	Lead ion	M	0.000E+00	7.782E-01	none	1.956E+04	0.000E+00
148	58-89-9	LINDANE	O	1.409E-04	none	3.040	7.300E+00	5.010E-06
149	330-55-2	LINURON	O	2.586E-07	none	2.813	7.500E+01	3.380E-06
150	106-42-3	M + P XYLENE	O	2.854E-01	none	2.763	2.286E+02	1.605E-04
151	14581-92-1	Magnesium ion	M	0.000E+00	0.000E+00	none	2.391E+03	0.000E+00
152	14333-14-3	Manganate	M	0.000E+00	6.902E-01	none	NoValueReported	0.000E+00
153	14302-87-5	Mercury ion	M	0.000E+00	1.716E+00	none	NoValueReported	0.000E+00
154	2032-65-7	METHIOCARB	O	4.882E-08	none	2.533	1.035E+02	6.418E-05
155	16752-77-5	METHOMYL	O	8.150E-10	none	0.212	5.800E+04	1.605E-04
156	72-43-5	METHOXYCHLOR	O	8.398E-06	none	4.693	3.020E-01	3.297E-06
157	78-93-3	METHYL ETHYL KETONE	O	1.937E-03	none	-0.097	2.400E+05	8.596E-05
158	80-62-6	METHYL METHACRYLATE	O	1.330E-02	none	0.993	1.600E+04	2.149E-05
159	1634-04-4	METHYL-T-BUTYL ETHER	O	2.428E-02	none	0.553	4.800E+04	3.343E-06
160	51218-45-2	METOLACHLOR	O	3.133E-08	none	2.513	8.640E+02	4.011E-05
161	21087-64-9	METRIBUZIN	O	4.840E-09	none	1.312	1.304E+03	6.418E-05
162	2212-67-1	MOLINATE	O	5.253E-05	none	1.699	9.700E+02	6.418E-05
163	108-90-7	MONOCHLOROBENZENE	O	none	none	none	none	none
164	108-38-3	M-XYLENE	O	2.970E-01	none	2.292	2.072E+02	3.343E-06
165	91-20-3	NAPHTHALENE	O	1.820E-02	none	2.913	1.421E+02	9.048E-06
166	104-51-8	N-BUTYLBENZENE	O	5.570E-01	none	3.480	1.608E+01	1.605E-04
167	14701-22-5	Nickel ion	M	0.000E+00	1.531E+00	none	2.395E+02	0.000E+00
168	14797-55-8	NITRATE	I	0.000E+00	-1.800E+01	none	NoValueReported	0.000E+00
169	none	NITRATE+NITRITE	I	0.000E+00	-1.800E+01	none	NoValueReported	0.000E+00
170	14797-65-0	NITRITE	I	0.000E+00	-1.800E+01	none	NoValueReported	0.000E+00
171	98-95-3	NITROBENZENE	O	8.563E-04	none	1.462	2.090E+03	3.054E-06
172	103-65-1	N-PROPYLBENZENE	O	4.240E-01	none	3.030	7.073E+01	1.605E-04
173	23120-99-2	Organotins	O	2.873E+00	none	-3.487	1.000E+06	8.023E-05
174	95-50-1	ORTHO-1,2-DICHLOROBENZENE	O	7.943E-02	none	2.840	1.500E+02	3.343E-06

CD	CAS	CONTAMINANT	TYPE	H	LogKd	LOGKOC	SOLUBILITY	Dg
175	23135-22-0	OXAMYL	O	1.600E-11	none	-0.866	2.800E+05	6.418E-05
176	95-47-6	O-XYLENE	O	2.140E-01	none	2.110	2.424E+02	3.343E-06
178	106-46-7	PARA-1,4-DICHLOROBENZENE	O	9.970E-02	none	2.810	9.024E+01	3.343E-06
179	53469-21-9	PCBs	O	7.860E-03	none	5.724	2.770E-01	1.605E-05
180	87-86-5	PENTACHLOROPHENOL	O	1.014E-06	none	2.613	1.400E+01	7.917E-07
181	14797-73-0	PERCHLORATE	I	0.000E+00	-1.800E+01	none	NoValueReported	0.000E+00
183	85-01-8	PHENANTHRENE	O	1.750E-03	none	4.072	1.150E+00	3.008E-06
184	1918-02-1	PICLORAM	O	2.205E-12	none	0.973	1.818E+03	4.011E-05
185	1610-18-0	PROMETON	O	3.700E-08	none	2.603	7.500E+02	4.011E-05
186	1918-16-7	PROPACHLOR	O	3.785E-06	none	1.793	7.000E+02	6.418E-05
187	139-40-2	PROPAZINE	O	1.903E-07	none	2.543	9.608E+01	4.011E-05
188	106-42-3	P-XYLENE	O	2.854E-01	none	2.490	2.286E+02	3.343E-06
189	129-00-0	PYRENE	O	4.573E-04	none	4.580	2.249E-01	3.167E-07
190	13982-63-3	RADIUM-226	I	0.000E+00	4.771E-01	none	NoValueReported	1.187E-06
191	15262-20-1	RADIUM-228	I	0.000E+00	4.771E-01	none	NoValueReported	2.374E-04
192	10043-92-2	Radon	I	4.395E+00	-1.800E+01	none	NoValueReported	1.733E-01
193	121-82-4	RDX	O	2.615E-06	none	0.483	6.062E+03	6.418E-05
194	135-98-8	S-BUTYLBENZENE	O	5.070E-01	none	3.320	1.810E+01	1.605E-04
195	7782-49-2	SELENIUM	M	0.000E+00	6.990E-01	none	NoValueReported	0.000E+00
196	14701-21-4	Silver ion	M	0.000E+00	4.314E-01	none	1.021E+04	0.000E+00
197	122-34-9	SIMAZINE	O	3.897E-08	none	1.793	5.899E+02	4.011E-05
198	17341-25-2	Sodium ion	M	0.000E+00	-1.800E+01	none	NoValueReported	0.000E+00
200	14701-18-9	Strontium ion	M	0.000E+00	0.000E+00	none	8.506E+03	1.373E-02
201	10098-97-2	STRONTIUM-90	M	0.000E+00	0.000E+00	none	8.506E+03	6.548E-05
202	100-42-5	STYRENE	O	1.138E-01	none	2.562	3.437E+02	5.730E-06
203	14808-79-8	SULFATE	I	0.000E+00	6.990E-01	none	NoValueReported	0.000E+00
204	98-06-6	T-BUTYLBENZENE	O	5.461E-01	none	3.390	2.734E+01	6.418E-05
206	5902-51-2	TERBACIL	O	4.964E-09	none	1.502	8.717E+02	6.418E-05
207	13071-79-9	TERBUFOS	O	9.929E-04	none	4.093	5.070E+00	6.418E-05
208	127-18-4	TETRACHLOROETHYLENE	O	7.322E-01	none	2.190	2.000E+02	1.671E-06
209	109-99-9	TETRAHYDROFURAN	O	2.917E-03	none	0.072	1.000E+06	1.605E-04
210	7440-28-0	THALLIUM	M	0.000E+00	-1.800E+01	none	NoValueReported	4.748E-04
211	108-88-3	TOLUENE	O	2.747E-01	none	2.146	5.731E+02	4.298E-05
212	7440-14-4	Radium Isotop	M	0.000E+00	4.771E-01	none	NoValueReported	1.187E-06
215	8001-35-2	TOXAPHENE	O	1.397E-04	none	4.981	7.400E-01	1.605E-05
216	156-60-5	TRANS-1,2-DICHLOROETHYLENE	O	1.688E-01	none	1.700	6.300E+03	6.418E-05
217	10061-02-6	TRANS-1,3-DICHLOROPROPENE	O	9.150E-02	none	1.642	2.800E+03	6.418E-05
218	122-34-9	TRIAZINES	O	3.897E-08	none	1.793	5.899E+02	4.011E-05
219	79-01-6	TRICHLOROETHYLENE	O	4.075E-01	none	1.970	1.280E+03	7.280E-07
220	75-69-4	TRICHLOROFLUOROMETHANE	O	4.013E+00	none	2.130	1.100E+03	1.671E-06

CD	CAS	CONTAMINANT	TYPE	H	LogKd	LOGKOC	SOLUBILITY	Dg
221	1582-09-8	TRIFLURALIN	O	2.012E-03	none	4.137	6.000E-01	1.605E-05
222	15086-10-9	TRITIUM	I	0.000E+00	-1.800E+01	none	NoValueReported	1.583E-04
223	none	URANIUM	M	0.000E+00	-3.979E-01	none	NoValueReported	4.220E-13
224	108-05-4	VINYL ACETATE	O	2.114E-02	none	0.342	3.025E+04	1.605E-04
225	75-01-4	VINYL CHLORIDE	O	1.150E+00	none	1.040	8.800E+03	4.186E-07
226	95-47-6	XYLENES (TOTAL)	O	2.140E-01	none	2.110	2.424E+02	3.343E-06
227	15176-26-8	Zinc ion	M	0.000E+00	-1.000E+00	none	3.192E+02	2.713E-03

APPENDIX 2 - ORIGINAL AND FINAL CAS NUMBERS AND CONTAMINANTS

The following table shows the original vs. final CAS numbers for the contaminants assessed in the Source Water Assessment Program. The method used for determining CAS numbers is presented in section 3.5.2.1.

Description of the fields

- CD – Identifier number of the contaminant.
- O_CAS – Original CAS number in the TRRP PCL table.
- O_CONTAMINANT – Original name in the TRRP PCL table
- FINAL_CAS – The final CAS number used in the dilution attenuation component.
- FINAL_CONTAMINANT - The final contaminant name used in the dilution attenuation component.

CD	O_CAS	O_CONTAMINANT	FINAL_CAS	FINAL_CONTAMINANT
1	630-20-6	1,1,1,2-TETRACHLOROETHANE	630-20-6	1,1,1,2-TETRACHLOROETHANE
2	71-55-6	1,1,1-TRICHLOROETHANE	71-55-6	1,1,1-TRICHLOROETHANE
3	79-34-5	1,1,2,2-TETRACHLOROETHANE	79-34-5	1,1,2,2-TETRACHLOROETHANE
4	79-00-5	1,1,2-TRICHLOROETHANE	79-00-5	1,1,2-TRICHLOROETHANE
5	75-34-3	1,1-DICHLOROETHANE	75-34-3	1,1-DICHLOROETHANE
6	75-35-4	1,1-DICHLOROETHYLENE	75-35-4	1,1-DICHLOROETHYLENE
7	563-58-6	1,1-DICHLOROPROPENE	563-58-6	1,1-DICHLOROPROPENE
8	87-61-6	1,2,3-TRICHLOROBENZENE	87-61-6	1,2,3-TRICHLOROBENZENE
9	96-18-4	1,2,3-TRICHLOROPROPANE	96-18-4	1,2,3-TRICHLOROPROPANE
10	120-82-1	1,2,4-TRICHLOROBENZENE	120-82-1	1,2,4-TRICHLOROBENZENE
11	95-63-6	1,2,4-TRIMETHYLBENZENE	95-63-6	1,2,4-TRIMETHYLBENZENE
12	107-06-2	1,2-DICHLOROETHANE	107-06-2	1,2-DICHLOROETHANE
13	78-87-5	1,2-DICHLOROPROPANE	78-87-5	1,2-DICHLOROPROPANE
14	122-66-7	1,2-DIPHENYLHYDRAZINE	122-66-7	1,2-DIPHENYLHYDRAZINE

CD	O_CAS	O_ CONTAMINANT	FINAL_CAS	FINAL_CONTAMINANT
15	108-67-8	1,3,5-TRIMETHYLBENZENE	108-67-8	1,3,5-TRIMETHYLBENZENE
16	541-73-1	1,3-DICHLOROBENZENE	541-73-1	1,3-DICHLOROBENZENE
17	142-28-9	1,3-DICHLOROPROPANE	142-28-9	1,3-DICHLOROPROPANE
18	542-75-6	1,3-DICHLOROPROPENE	542-75-6	1,3-DICHLOROPROPENE
19	594-83-2	2,2-DICHLOROPROPANE	594-20-7	2,2-DICHLOROPROPANE
20	1746-01-6	2,3,7,8-TCDD	1746-01-6	2,3,7,8-TCDD
21	93-76-5	2,4,5-T	93-76-5	2,4,5-T
22	93-72-1	2,4,5-TP	93-72-1	2,4,5-TP
23	88-06-2	2,4,6-TRICHLOROPHENOL	88-06-2	2,4,6-TRICHLOROPHENOL
24	94-75-7	2,4-D	94-75-7	2,4-D
25	120-83-2	2,4-DICHLOROPHENOL	120-83-2	2,4-DICHLOROPHENOL
26	51-28-5	2,4-DINITROPHENOL	51-28-5	2,4-DINITROPHENOL
27	121-14-2	2,4-DINITROTOLUENE	121-14-2	2,4-DINITROTOLUENE
28	606-20-2	2,6-DINITROTOLUENE	606-20-2	2,6-DINITROTOLUENE
29	95-49-8	2-CHLOROTOLUENE	95-49-8	2-CHLOROTOLUENE
30	591-78-6	2-HEXANONE	591-78-6	2-HEXANONE
31	95-48-7	2-METHYLPHENOL	95-48-7	2-METHYLPHENOL
32	16655-82-6	3-HYDROXYCARBOFURAN	16655-82-6	3-HYDROXYCARBOFURAN
33	106-43-4	4-CHLOROTOLUENE	106-43-4	4-CHLOROTOLUENE
34	99-87-6	4-ISOPROPYLTOLUENE	99-87-6	4-ISOPROPYLTOLUENE
35	108-10-1	4-METHYL-2-PENTANONE	108-10-1	4-METHYL-2-PENTANONE
36	83-32-9	ACENAPHTHENE	83-32-9	ACENAPHTHENE
37	208-96-8	ACENAPHTHYLENE	208-96-8	ACENAPHTHYLENE
38	34256-82-1	ACETOCHLOR	34256-82-1	ACETOCHLOR
39	67-64-1	ACETONE	67-64-1	ACETONE
40	107-13-1	ACRYLONITRILE	107-13-1	ACRYLONITRILE
41	15972-60-8	ALACHLOR	15972-60-8	ALACHLOR
42	116-06-3	ALDICARB	116-06-3	ALDICARB
43	1646-88-4	ALDICARB SULFONE	1646-88-4	ALDICARB SULFONE
44	1646-87-3	ALDICARB SULFOXIDE	1646-87-3	ALDICARB SULFOXIDE
45	309-00-2	ALDRIN	309-00-2	ALDRIN
46	NONE	ALKALINITY	NOT EVALUATED	ALKALINITY
47	7429-90-5	ALUMINUM	14903-36-7	ALUMINUM CATION
48	120-12-7	ANTHRACENE	120-12-7	ANTHRACENE
49	7440-36-0	ANTIMONY	64924-52-3	ANTIMONATE
50	NONE	AROCLOR	53469-21-9	AROCLOR
51	7440-38-2	ARSENIC	15584-04-0	ARSENATE
52	1332-21-4	ASBESTOS	1332-21-4	ASBESTOS
53	1912-24-9	ATRAZINE	1912-24-9	ATRAZINE
54	7440-39-3	BARIUM	16541-35-8	BARIUM CATION

CD	O_CAS	O_ CONTAMINANT	FINAL_CAS	FINAL_CONTAMINANT
55	25057-89-0	BENTAZON	25057-89-0	BENTAZON
56	71-43-2	BENZENE	71-43-2	BENZENE
57	56-55-3	BENZO(A)ANTHRACENE	56-55-3	BENZO(A)ANTHRACENE
58	50-32-8	BENZO(A)PYRENE	50-32-8	BENZO(A)PYRENE
59	205-99-2	BENZO(B)FLUORANTHENE	205-99-2	BENZO(B)FLUORANTHENE
60	191-24-2	BENZO(G,H,I)PERYLENE	191-24-2	BENZO(G,H,I)PERYLENE
61	207-08-9	BENZO(K)FLUORANTHENE	207-08-9	BENZO(K)FLUORANTHENE
62	7440-41-7	BERYLLIUM	14701-08-7	BERYLLIUM ION
63	71-52-3	BICARBONATE	71-52-3	BICARBONATE
64	7440-42-8	BORON	11113-50-1	BORIC ACID
65	314-40-9	BROMACIL	314-40-9	BROMACIL
66	NONE	BROMIDE	24959-67-9	BROMIDE
67	108-86-1	BROMOBENZENE	108-86-1	BROMOBENZENE
68	74-97-5	BROMOCHLOROMETHANE	74-97-5	BROMOCHLOROMETHANE
69	75-27-4	BROMODICHLOROMETHANE	75-27-4	BROMODICHLOROMETHANE
70	75-25-2	BROMOFORM	75-25-2	BROMOFORM
71	74-83-9	BROMOMETHANE	74-83-9	BROMOMETHANE
72	23184-66-9	BUTACHLOR	23184-66-9	BUTACHLOR
73	85-68-7	BUTYL BENZYL PHTHALATE	85-68-7	BUTYL BENZYL PHTHALATE
74	7440-43-9	CADMIUM	22537-48-0	CADMIUM CATION
75	7440-70-2	CALCIUM	14102-48-8	CALCIUM CATION
76	63-25-2	CARBARYL	63-25-2	CARBARYL
77	1563-66-2	CARBOFURAN	1563-66-2	CARBOFURAN
78	75-15-0	CARBON DISULFIDE	75-15-0	CARBON DISULFIDE
79	56-23-5	CARBON TETRACHLORIDE	56-23-5	CARBON TETRACHLORIDE
80	3812-32-6	CARBONATE	3812-32-6	CARBONATE
81	57-74-9	CHLORDANE	57-74-9	CHLORDANE
82	5103-71-9	CHLORDANE (ALPHA-CHLORDANE)	5103-71-9	CHLORDANE (ALPHA-CHLORDANE)
83	12789-03-6	CHLORDANE (GAMMA-CHLORDANE)	12789-03-6	CHLORDANE (GAMMA-CHLORDANE)
84	39765-80-5	CHLORDANE (TRANS-NONACHLOR)	39765-80-5	CHLORDANE (TRANS-NONACHLOR)
85	68188-88-5	CHLORIDE	16887-00-6	CHLORIDE
86	108-90-7	CHLOROBENZENE	108-90-7	CHLOROBENZENE
87	75-00-3	CHLOROETHANE	75-00-3	CHLOROETHANE
88	67-66-3	CHLOROFORM	67-66-3	CHLOROFORM
89	74-87-3	CHLOROMETHANE	74-87-3	CHLOROMETHANE
90	7440-47-3	CHROMIUM	11104-59-9	CHROMATE
91	218-01-9	CHRYSENE	218-01-9	CHRYSENE
92	156-59-2	CIS-1,2-DICHLOROETHYLENE	156-59-2	CIS-1,2-DICHLOROETHYLENE
93	10061-01-5	CIS-1,3-DICHLOROPROPENE	10061-01-5	CIS-1,3-DICHLOROPROPENE
94	7440-50-8	COPPER	17493-86-6	COPPER ION

CD	O_CAS	O_ CONTAMINANT	FINAL_CAS	FINAL_CONTAMINANT
95	NONE	CRYPTOSPORIDIUM PARVUM	NOT EVALUATED	CRYPTOSPORIDIUM PARVUM
96	21725-46-2	CYANAZINE	21725-46-2	CYANAZINE
97	57-12-5	CYANIDE	57-12-5	CYANIDE
98	75-99-0	DALAPON	75-99-0	DALAPON
99	NONE	DCPA DI-ACID DEGRADATE	2136-79-0	DCPA DI-ACID DEGRADATE
100	NONE	DCPA MONO-ACID DEGRADATE	887-54-7	DCPA MONO-ACID DEGRADATE
101	72-55-9	DDE	72-55-9	DDE
102	103-23-1	DI-(2-ETHYLHEXYL)ADIPATE	103-23-1	DI-(2-ETHYLHEXYL)ADIPATE
103	117-81-7	DI-(2-ETHYLHEXYL)PHTHALATE	117-81-7	DI-(2-ETHYLHEXYL)PHTHALATE
104	333-41-5	DIAZINON	333-41-5	DIAZINON
105	53-70-3	DIBENZ(A,H)ANTHRACENE	53-70-3	DIBENZ(A,H)ANTHRACENE
106	124-48-1	DIBROMOCHLOROMETHANE	124-48-1	DIBROMOCHLOROMETHANE
107	67708-83-2	DIBROMOCHLOROPROPANE	67708-83-2	DIBROMOCHLOROPROPANE
108	74-95-3	DIBROMOMETHANE	74-95-3	DIBROMOMETHANE
109	1918-00-9	DICAMBA	1918-00-9	DICAMBA
110	75-71-8	DICHLORODIFLUOROMETHANE	75-71-8	DICHLORODIFLUOROMETHANE
111	75-09-2	DICHLOROMETHANE	75-09-2	DICHLOROMETHANE
112	60-57-1	DIELDRIN	60-57-1	DIELDRIN
113	84-66-2	DIETHYL PHTHALATE	84-66-2	DIETHYL PHTHALATE
114	131-11-3	DIMETHYL PHTHALATE	131-11-3	DIMETHYL PHTHALATE
115	84-74-2	DI-N-BUTYL PHTHALATE	84-74-2	DI-N-BUTYL PHTHALATE
116	88-85-7	DINOSEB	88-85-7	DINOSEB
117	2764-72-9	DIQUAT	2764-72-9	DIQUAT
118	298-04-4	DISULFOTON	298-04-4	DISULFOTON
119	330-54-1	DIURON	330-54-1	DIURON
120	145-73-3	ENDOTHALL	145-73-3	ENDOTHALL
121	72-20-8	ENDRIN	72-20-8	ENDRIN
122	759-94-4	EPTC	759-94-4	EPTC
123	NONE	ESCHERICHIA COLI	NOT EVALUATED	ESCHERICHIA COLI
124	97-63-2	ETHYL METHACRYLATE	97-63-2	ETHYL METHACRYLATE
125	100-41-4	ETHYLBENZENE	100-41-4	ETHYLBENZENE
126	106-93-4	ETHYLENE DIBROMIDE	106-93-4	ETHYLENE DIBROMIDE
127	NONE	FECAL VIRUSES	NOT EVALUATED	FECAL VIRUSES
128	86-73-7	FLUORENE	86-73-7	FLUORENE
129	16984-48-8	FLUORIDE	16984-48-8	FLUORIDE
130	944-22-9	FONOFOS	944-22-9	FONOFOS
131	NONE	GIARDIA LAMBLIA	NOT EVALUATED	GIARDIA LAMBLIA
132	1071-83-6	GLYPHOSATE	1071-83-6	GLYPHOSATE

CD	O_CAS	O_ CONTAMINANT	FINAL_CAS	FINAL_CONTAMINANT
133	NONE	GROSS ALPHA	NOT EVALUATED	GROSS ALPHA
134	NONE	GROSS BETA	NOT EVALUATED	GROSS BETA
135	NONE	HARDNESS	NOT EVALUATED	HARDNESS
136	76-44-8	HEPTACHLOR	76-44-8	HEPTACHLOR
137	1024-57-3	HEPTACHLOR EPOXIDE	1024-57-3	HEPTACHLOR EPOXIDE
138	118-74-1	HEXACHLOROBENZENE	118-74-1	HEXACHLOROBENZENE
139	87-68-3	HEXACHLOROBUTADIENE	87-68-3	HEXACHLOROBUTADIENE
140	77-47-4	HEXACHLOROCYCLOPENTADIENE	77-47-4	HEXACHLOROCYCLOPENTADIENE
141	7783-06-4	HYDROGEN SULFIDE	15035-72-0	SULFIDE
142	193-39-5	INDENO[1,2,3,CD]PYRENE	193-39-5	INDENO[1,2,3,CD]PYRENE
143	74-88-4	IODOMETHANE	74-88-4	IODOMETHANE
144	7439-89-6	IRON	15438-31-0	IRON ION
145	98-82-8	ISOPROPYLBENZENE	98-82-8	ISOPROPYLBENZENE
146	845-52-3	LAMBAST	845-52-3	LAMBAST
147	7439-92-1	LEAD	14701-27-0	LEAD ION
148	58-89-9	LINDANE	58-89-9	LINDANE
149	330-55-2	LINURON	330-55-2	LINURON
150	NONE	M + P XYLENE	106-42-3	P XYLENE
151	7439-95-4	MAGNESIUM	14581-92-1	MAGNESIUM ION
152	7439-96-5	MANGANESE	14333-14-3	MANGANATE
153	7439-97-6	MERCURY	14302-87-5	MERCURY ION
154	2032-65-7	METHIOCARB	2032-65-7	METHIOCARB
155	16752-77-5	METHOMYL	16752-77-5	METHOMYL
156	72-43-5	METHOXYCHLOR	72-43-5	METHOXYCHLOR
157	78-93-3	METHYL ETHYL KETONE	78-93-3	METHYL ETHYL KETONE
158	80-62-6	METHYL METHACRYLATE	80-62-6	METHYL METHACRYLATE
159	1634-04-4	METHYL-T-BUTYL ETHER	1634-04-4	METHYL-T-BUTYL ETHER
160	51218-45-2	METOLACHLOR	51218-45-2	METOLACHLOR
161	21087-64-9	METRIBUZIN	21087-64-9	METRIBUZIN
162	2212-67-1	MOLINATE	2212-67-1	MOLINATE
163	NONE	MONOCHLOROBENZENE	108-90-7	MONOCHLOROBENZENE
164	108-38-3	M-XYLENE	108-38-3	M-XYLENE
165	91-20-3	NAPHTHALENE	91-20-3	NAPHTHALENE
166	104-51-8	N-BUTYLBENZENE	104-51-8	N-BUTYLBENZENE
167	7440-02-0	NICKEL	14701-22-5	NICKEL ION
168	14797-55-8	NITRATE	14797-55-8	NITRATE
169	NONE	NITRATE+NITRITE	NOTEVALUATED	NITRATE+NITRITE
170	14797-65-0	NITRITE	14797-65-0	NITRITE
171	98-95-3	NITROBENZENE	98-95-3	NITROBENZENE

CD	O_CAS	O_ CONTAMINANT	FINAL_CAS	FINAL_CONTAMINANT
172	103-65-1	N-PROPYLBENZENE	103-65-1	N-PROPYLBENZENE
173	NONE	ORGANOTINS	23120-99-2	ORGANOTINS
174	95-50-1	ORTHO-1,2-DICHLOROBENZENE	95-50-1	ORTHO-1,2-DICHLOROBENZENE
175	23135-22-0	OXAMYL	23135-22-0	OXAMYL
176	95-47-6	O-XYLENE	95-47-6	O-XYLENE
177	NONE	P ALKALINITY	NOTEVALUATED	P ALKALINITY
178	106-46-7	PARA-1,4-DICHLOROBENZENE	106-46-7	PARA-1,4-DICHLOROBENZENE
179	NONE	PCBS	53469-21-9	PCBS
180	87-86-5	PENTACHLOROPHENOL	87-86-5	PENTACHLOROPHENOL
181	14797-73-0	PERCHLORATE	14797-73-0	PERCHLORATE
182	NONE	PH	NOTEVALUATED	PH
183	85-01-8	PHENANTHRENE	85-01-8	PHENANTHRENE
184	1918-02-1	PICLORAM	1918-02-1	PICLORAM
185	1610-18-0	PROMETON	1610-18-0	PROMETON
186	1918-16-7	PROPACHLOR	1918-16-7	PROPACHLOR
187	139-40-2	PROPAZINE	139-40-2	PROPAZINE
188	106-42-3	P-XYLENE	106-42-3	P-XYLENE
189	129-00-0	PYRENE	129-00-0	PYRENE
190	15262-20-1	RADIUM-226	13982-63-3	NONE
191	13982-63-3	RADIUM-228	15262-20-1	NONE
192	10043-92-2	RADON	10043-92-2	RADON
193	121-82-4	RDX	121-82-4	RDX
194	135-98-8	S-BUTYLBENZENE	135-98-8	S-BUTYLBENZENE
195	7782-49-2	SELENIUM	7782-49-2	SELENIUM
196	7440-22-4	SILVER	14701-21-4	SILVER ION
197	122-34-9	SIMAZINE	122-34-9	SIMAZINE
198	7440-23-5	SODIUM	17341-25-2	SODIUM ION
199	NONE	SPECIFIC CONDUCTANCE	NOTEVALUATED	SPECIFIC CONDUCTANCE
200	14158-27-1	STRONTIUM-89	14701-18-9	STRONTIUM ION
201	10098-97-2	STRONTIUM-90	10098-97-2	STRONTIUM-90
202	100-42-5	STYRENE	100-42-5	STYRENE
203	14808-79-8	SULFATE	14808-79-8	SULFATE
204	98-06-6	T-BUTYLBENZENE	98-06-6	T-BUTYLBENZENE
205	NONE	TDS	NOTEVALUATED	TDS
206	5902-51-2	TERBACIL	5902-51-2	TERBACIL
207	13071-79-9	TERBUFOS	13071-79-9	TERBUFOS
208	127-18-4	TETRACHLOROETHYLENE	127-18-4	TETRACHLOROETHYLENE
209	109-99-9	TETRAHYDROFURAN	109-99-9	TETRAHYDROFURAN
210	7440-28-0	THALLIUM	7440-28-0	THALLIUM
211	108-88-3	TOLUENE	108-88-3	TOLUENE

CD	O_CAS	O_ CONTAMINANT	FINAL_CAS	FINAL_CONTAMINANT
212	NONE	TOTAL ALPHA EMITTING RADIUM	7440-14-4	RADIUM ISOTOP
213	NONE	TOTAL COLIFORM	NOTEVALUATED	TOTAL COLIFORM
214	NONE	TOTAL TRIHALOMETHANES	NOTEVALUATED	NONE
215	8001-35-2	TOXAPHENE	8001-35-2	TOXAPHENE
216	156-60-5	TRANS-1,2-DICHLOROETHYLENE	156-60-5	TRANS-1,2-DICHLOROETHYLENE
217	10061-02-6	TRANS-1,3-DICHLOROPROPENE	10061-02-6	TRANS-1,3-DICHLOROPROPENE
218	NONE	TRIAZINES	122-34-9	TRIAZINES
219	79-01-6	TRICHLOROETHYLENE	79-01-6	TRICHLOROETHYLENE
220	75-69-4	TRICHLOROFLUOROMETHANE	75-69-4	TRICHLOROFLUOROMETHANE
221	1582-09-8	TRIFLURALIN	1582-09-8	TRIFLURALIN
222	10028-17-8	TRITIUM	15086-10-9	TRITIUM
223	NONE	URANIUM	NONE	NONE
224	108-05-4	VINYL ACETATE	108-05-4	VINYL ACETATE
225	75-01-4	VINYL CHLORIDE	75-01-4	VINYL CHLORIDE
226	NONE	XYLENES (TOTAL)	95-47-6	XYLENES (TOTAL)
227	7440-66-6	ZINC	15176-26-8	ZINC ION

APPENDIX 3 - PARTITION COEFFICIENTS FOR ORGANIC COMPOUNDS

The following table shows the partitioning coefficients selected for the contaminants. A more detailed description of the sources of information and selection methods is presented in section 3.5.2.3

Description of the fields

- CD – Identifier number of the contaminant.
- FINAL_CAS – The final CAS number used in the dilution attenuation component.
- FINAL_CONTAMINANT - The final contaminant name used in the dilution attenuation component.
- TYPE – the type of the contaminant, organic, inorganic or metal.
- H – Selected Henry's law constant (dimensionless).
- LOG KOC – The log of selected Koc values (cm^3-water/g-carbon).
- SOLUBILITY - Selected solubility value (mg/l).

Description of the colors

The colors below relate the selected values for partition coefficients with their source of information.

EPI Suite software
TRRP PCL table
PhysPro

CD	FINAL_CAS	FINAL_CONTAMINANT	TYPE	H	LOG KOC	SOLUBILITY
1	630-20-6	1,1,1,2-TETRACHLOROETHANE	O	9.977E-02	2.543	1.100E+03
2	71-55-6	1,1,1-TRICHLOROETHANE	O	7.116E-01	2.040	1.330E+03
3	79-34-5	1,1,2,2-TETRACHLOROETHANE	O	1.518E-02	1.890	2.970E+03
4	79-00-5	1,1,2-TRICHLOROETHANE	O	3.409E-02	1.502	4.420E+03
5	75-34-3	1,1-DICHLOROETHANE	O	2.325E-01	1.403	5.500E+03
6	75-35-4	1,1-DICHLOROETHYLENE	O	1.056E+00	1.743	2.400E+03
7	563-58-6	1,1-DICHLOROPROPENE	O	1.819E+00	2.143	7.488E+02
8	87-61-6	1,2,3-TRICHLOROBENZENE	O	3.800E-02	3.663	1.884E+01
9	96-18-4	1,2,3-TRICHLOROPROPANE	O	1.419E-02	1.883	1.900E+03
10	120-82-1	1,2,4-TRICHLOROBENZENE	O	5.874E-02	3.220	4.880E+01
11	95-63-6	1,2,4-TRIMETHYLBENZENE	O	1.840E-01	2.970	7.959E+01
12	107-06-2	1,2-DICHLOROETHANE	O	4.882E-02	1.093	8.700E+03
13	78-87-5	1,2-DICHLOROPROPANE	O	1.168E-01	1.593	2.800E+03
14	122-66-7	1,2-DIPHENYLHYDRAZINE	O	1.422E-07	2.553	1.840E+03
15	108-67-8	1,3,5-TRIMETHYLBENZENE	O	2.720E-01	3.010	5.148E+01
16	541-73-1	1,3-DICHLOROBENZENE	O	1.088E-01	2.230	1.100E+02
17	142-28-9	1,3-DICHLOROPROPANE	O	4.038E-02	1.613	2.157E+03
18	542-75-6	1,3-DICHLOROPROPENE	O	1.226E-01	1.642	1.994E+03
19	594-20-7	2,2-DICHLOROPROPANE	O	3.394E-01	2.192	1.682E+03
20	1746-01-6	2,3,7,8-TCDD	O	1.474E-03	6.413	1.103E-03
21	93-76-5	2,4,5-T	O	2.826E-07	2.474	2.780E+02
22	93-72-1	2,4,5-TP	O	3.748E-07	3.413	1.400E+02
23	88-06-2	2,4,6-TRICHLOROPHENOL	O	1.076E-04	2.117	9.820E+02
24	94-75-7	2,4-D	O	5.820E-09	2.423	8.900E+02
25	120-83-2	2,4-DICHLOROPHENOL	O	9.060E-05	1.857	4.500E+03
26	51-28-5	2,4-DINITROPHENOL	O	2.012E-07	-2.000	5.800E+03
27	121-14-2	2,4-DINITROTOLUENE	O	2.234E-06	1.593	4.462E+02
28	606-20-2	2,6-DINITROTOLUENE	O	3.090E-05	1.620	3.524E+02
29	95-49-8	2-CHLOROTOLUENE	O	1.347E-01	2.610	1.540E+02
30	591-78-6	2-HEXANONE	O	3.381E-03	0.993	1.794E+04
31	95-48-7	2-METHYLPHENOL	O	4.964E-05	1.562	2.040E+04
32	16655-82-6	3-HYDROXYCARBOFURAN	O	2.466E-12	0.373	6.207E+03
33	106-43-4	4-CHLOROTOLUENE	O	1.335E-01	2.696	1.358E+02

CD	FINAL_CAS	FINAL_CONTAMINANT	TYPE	H	LOG KOC	SOLUBILITY
34	99-87-6	4-ISOPROPYLTOLUENE	O	4.551E-01	3.360	2.788E+01
35	108-10-1	4-METHYL-2-PENTANONE	O	5.709E-03	0.923	1.900E+04
36	83-32-9	ACENAPHTHENE	O	6.443E-03	3.533	4.240E+00
37	208-96-8	ACENAPHTHYLENE	O	4.739E-03	3.553	3.930E+00
38	34256-82-1	ACETOCHLOR	O	9.225E-07	2.642	2.230E+02
39	67-64-1	ACETONE	O	1.613E-03	-0.627	6.000E+05
40	107-13-1	ACRYLONITRILE	O	5.709E-03	-0.137	7.500E+04
41	15972-60-8	ALACHLOR	O	3.442E-07	2.279	2.400E+02
42	116-06-3	ALDICARB	O	5.820E-08	0.743	6.000E+03
43	1646-88-4	ALDICARB SULFONE	O	1.096E-07	-0.959	8.000E+03
44	1646-87-3	ALDICARB SULFOXIDE	O	4.009E-08	-1.167	2.800E+04
45	309-00-2	ALDRIN	O	1.820E-03	4.680	7.840E-02
48	120-12-7	ANTHRACENE	O	2.300E-03	4.064	6.905E-01
50	53469-21-9	AROCLOR	O	7.860E-03	5.903	2.770E-01
53	1912-24-9	ATRAZINE	O	9.763E-08	2.204	2.141E+02
55	25057-89-0	BENTAZON	O	9.019E-08	1.953	5.000E+02
56	71-43-2	BENZENE	O	2.274E-01	1.743	2.000E+03
57	56-55-3	BENZO(A)ANTHRACENE	O	1.393E-04	5.373	2.907E-02
58	50-32-8	BENZO(A)PYRENE	O	1.891E-05	5.740	1.038E-02
59	205-99-2	BENZO(B)FLUORANTHENE	O	2.718E-05	5.393	2.065E-02
60	191-24-2	BENZO(G,H,I)PERYLENE	O	1.369E-05	6.200	2.842E-03
61	207-08-9	BENZO(K)FLUORANTHENE	O	4.448E-07	5.723	1.079E-02
65	314-40-9	BROMACIL	O	4.344E-09	1.723	8.150E+02
67	108-86-1	BROMOBENZENE	O	8.382E-02	2.384	4.460E+02
68	74-97-5	BROMOCHLOROMETHANE	O	3.690E-02	1.021	2.042E+04
69	75-27-4	BROMODICHLOROMETHANE	O	8.770E-02	1.613	4.500E+03
70	75-25-2	BROMOFORM	O	2.213E-02	1.940	3.200E+03
71	74-83-9	BROMOMETHANE	O	2.581E-01	0.803	1.520E+04
72	23184-66-9	BUTACHLOR	O	2.110E-06	4.114	2.300E+01
73	85-68-7	BUTYL BENZYL PHTHALATE	O	5.213E-05	4.138	2.900E+00
76	63-25-2	CARBARYL	O	1.804E-07	1.973	4.162E+02
77	1563-66-2	CARBOFURAN	O	1.278E-07	1.462	7.000E+02
78	75-15-0	CARBON DISULFIDE	O	5.957E-01	1.553	2.928E+03

CD	FINAL_CAS	FINAL_CONTAMINANT	TYPE	H	LOG KOC	SOLUBILITY
79	56-23-5	CARBON TETRACHLORIDE	O	1.142E+00	2.270	8.050E+02
81	57-74-9	CHLORDANE	O	2.011E-03	5.080	5.600E-02
82	5103-71-9	CHLORDANE (ALPHA-CHLORDANE)	O	2.011E-03	5.833	4.640E-02
83	12789-03-6	CHLORDANE (GAMMA-CHLORDANE)	O	2.011E-03	5.833	1.299E-02
84	39765-80-5	CHLORDANE (TRANS-NONACHLOR)	O	1.026E-03	5.963	6.120E-03
86	108-90-7	CHLOROBENZENE	O	1.287E-01	2.330	5.020E+02
87	75-00-3	CHLOROETHANE	O	2.120E-01	1.041	2.000E+04
88	67-66-3	CHLOROFORM	O	1.518E-01	1.583	7.920E+03
89	74-87-3	CHLOROMETHANE	O	3.649E-01	0.522	2.262E+04
91	218-01-9	CHRYSENE	O	5.030E-05	5.423	2.635E-02
92	156-59-2	CIS-1,2-DICHLOROETHYLENE	O	1.688E-01	1.462	6.410E+03
93	10061-01-5	CIS-1,3-DICHLOROPROPENE	O	9.150E-02	1.642	2.700E+03
96	21725-46-2	CYANAZINE	O	1.225E-10	1.692	1.838E+02
98	75-99-0	DALAPON	O	3.732E-06	1.292	5.020E+05
99	2136-79-0	DCPA DI-ACID DEGRADATE	O	8.398E-12	1.743	1.754E+02
100	887-54-7	DCPA MONO-ACID DEGRADATE	O	3.351E-09	2.803	1.826E+01
101	72-55-9		O	8.730E-04	5.040	6.500E-02
102	103-23-1	DI-(2-ETHYLHEXYL)ADIPATE	O	1.795E-05	5.580	7.800E-01
103	117-81-7	DI-(2-ETHYLHEXYL)PHTHALATE	O	1.117E-05	7.212	3.000E-01
104	333-41-5	DIAZINON	O	4.675E-06	2.120	4.000E+01
105	53-70-3	DIBENZ(A,H)ANTHRACENE	O	4.656E-07	6.152	3.304E-03
106	124-48-1	DIBROMOCHLOROMETHANE	O	3.239E-02	1.770	5.250E+03
107	67708-83-2	DIBROMOCHLOROPROPANE	O	6.081E-03	2.230	1.000E+03
108	74-95-3	DIBROMOMETHANE	O	3.401E-02	1.312	1.100E+04
109	1918-00-9	DICAMBA	O	9.019E-08	0.342	8.310E+03
110	75-71-8	DICHLORODIFLUOROMETHANE	O	1.419E+01	1.773	2.800E+02
111	75-09-2	DICHLOROMETHANE	O	9.104E-02	0.863	1.540E+04
112	60-57-1	DIELDRIN	O	1.110E-04	4.330	1.950E-01
113	84-66-2	DIETHYL PHTHALATE	O	1.871E-05	2.033	1.080E+03
114	131-11-3	DIMETHYL PHTHALATE	O	4.344E-06	1.500	4.190E+03
115	84-74-2	DI-N-BUTYL PHTHALATE	O	5.945E-05	4.114	1.120E+01
116	88-85-7	DINOSEB	O	1.886E-05	3.080	5.200E+01
117	2764-72-9	DIQUAT	O	2.690E-12	1.973	7.000E+01

CD	FINAL_CAS	FINAL_CONTAMINANT	TYPE	H	LOG KOC	SOLUBILITY
118	298-04-4	DISULFOTON	O	8.936E-05	3.632	1.600E+01
119	330-54-1	DIURON	O	2.085E-08	2.292	1.506E+02
120	145-73-3	ENDOTHALL	O	1.593E-14	1.522	1.000E+05
121	72-20-8	ENDRIN	O	4.947E-05	3.970	2.500E-01
122	759-94-4	EPTC	O	6.578E-04	2.823	3.700E+02
124	97-63-2	ETHYL METHACRYLATE	O	6.651E-03	1.553	1.900E+04
125	100-41-4	ETHYLBENZENE	O	3.260E-01	2.310	2.286E+02
126	106-93-4	ETHYLENE DIBROMIDE	O	2.759E-02	1.573	4.320E+03
128	86-73-7	FLUORENE	O	2.644E-03	3.793	1.980E+00
130	944-22-9	FONOFOS	O	2.888E-04	3.553	1.070E+01
132	1071-83-6	GLYPHOSATE	O	1.688E-17	-4.387	1.000E+06
136	76-44-8	HEPTACHLOR	O	1.216E-02	4.070	1.800E-01
137	1024-57-3	HEPTACHLOR EPOXIDE	O	3.446E-04	3.859	2.750E-01
138	118-74-1	HEXACHLOROBENZENE	O	2.224E-02	4.450	1.922E-01
139	87-68-3	HEXACHLOROBUTADIENE	O	4.261E-01	3.840	3.200E+00
140	77-47-4	HEXACHLOROCYCLOPENTADIENE	O	7.150E-01	3.980	1.800E+00
142	193-39-5	INDENO[1,2,3,CD]PYRENE	O	2.852E-06	6.312	3.751E-03
143	74-88-4	IODOMETHANE	O	2.176E-01	1.124	1.244E+04
145	98-82-8	ISOPROPYLBENZENE	O	4.757E-01	3.272	7.503E+01
146	845-52-3	LAMBAST	O	5.171E-11	1.963	1.188E+02
148	58-89-9	LINDANE	O	1.409E-04	3.040	7.300E+00
149	330-55-2	LINURON	O	2.586E-07	2.813	7.500E+01
150	106-42-3	M + P XYLENE	O	2.854E-01	2.763	2.286E+02
154	2032-65-7	METHIOCARB	O	4.882E-08	2.533	1.035E+02
155	16752-77-5	METHOMYL	O	8.150E-10	0.212	5.800E+04
156	72-43-5	METHOXYCHLOR	O	8.398E-06	4.693	3.020E-01
157	78-93-3	METHYL ETHYL KETONE	O	1.937E-03	-0.097	2.400E+05
158	80-62-6	METHYL METHACRYLATE	O	1.330E-02	0.993	1.600E+04
159	1634-04-4	METHYL-T-BUTYL ETHER	O	2.428E-02	0.553	4.800E+04
160	51218-45-2	METOLACHLOR	O	3.133E-08	2.513	8.640E+02
161	21087-64-9	METRIBUZIN	O	4.840E-09	1.312	1.304E+03
162	2212-67-1	MOLINATE	O	5.253E-05	1.699	9.700E+02
164	108-38-3	M-XYLENE	O	2.970E-01	2.292	2.072E+02
165	91-20-3	NAPHTHALENE	O	1.820E-02	2.913	1.421E+02

CD	FINAL_CAS	FINAL_CONTAMINANT	TYPE	H	LOG KOC	SOLUBILITY
166	104-51-8	N-BUTYLBENZENE	O	5.570E-01	3.480	1.608E+01
171	98-95-3	NITROBENZENE	O	8.563E-04	1.462	2.090E+03
172	103-65-1	N-PROPYLBENZENE	O	4.240E-01	3.030	7.073E+01
173	23120-99-2	Organotins	O	2.873E+00	-3.487	1.000E+06
174	95-50-1	ORTHO-1,2-DICHLOROBENZENE	O	7.943E-02	2.840	1.500E+02
175	23135-22-0	OXAMYL	O	1.600E-11	-0.866	2.800E+05
176	95-47-6	O-XYLENE	O	2.140E-01	2.110	2.424E+02
178	106-46-7	PARA-1,4-DICHLOROBENZENE	O	9.970E-02	2.810	9.024E+01
179	53469-21-9	PCBs	O	7.860E-03	5.724	2.770E-01
180	87-86-5	PENTACHLOROPHENOL	O	1.014E-06	2.613	1.400E+01
183	85-01-8	PHENANTHRENE	O	1.750E-03	4.072	1.150E+00
184	1918-02-1	PICLORAM	O	2.205E-12	0.973	1.818E+03
185	1610-18-0	PROMETON	O	3.700E-08	2.603	7.500E+02
186	1918-16-7	PROPACHLOR	O	3.785E-06	1.793	7.000E+02
187	139-40-2	PROPAZINE	O	1.903E-07	2.543	9.608E+01
188	106-42-3	P-XYLENE	O	2.854E-01	2.490	2.286E+02
189	129-00-0	PYRENE	O	4.573E-04	4.580	2.249E-01
193	121-82-4	RDX	O	2.615E-06	0.483	6.062E+03
194	135-98-8	S-BUTYLBENZENE	O	5.070E-01	3.320	1.810E+01
197	122-34-9	SIMAZINE	O	3.897E-08	1.793	5.899E+02
202	100-42-5	STYRENE	O	1.138E-01	2.562	3.437E+02
204	98-06-6	T-BUTYLBENZENE	O	5.461E-01	3.390	2.734E+01
206	5902-51-2	TERBACIL	O	4.964E-09	1.502	8.717E+02
207	13071-79-9	TERBUFOS	O	9.929E-04	4.093	5.070E+00
208	127-18-4	TETRACHLOROETHYLENE	O	7.322E-01	2.190	2.000E+02
209	109-99-9	TETRAHYDROFURAN	O	2.917E-03	0.072	1.000E+06
211	108-88-3	TOLUENE	O	2.747E-01	2.146	5.731E+02
215	8001-35-2	TOXAPHENE	O	1.397E-04	4.981	7.400E-01
216	156-60-5	TRANS-1,2-DICHLOROETHYLENE	O	1.688E-01	1.700	6.300E+03
217	10061-02-6	TRANS-1,3-DICHLOROPROPENE	O	9.150E-02	1.642	2.800E+03
218	122-34-9	TRIAZINES	O	3.897E-08	1.793	5.899E+02
219	79-01-6	TRICHLOROETHYLENE	O	4.075E-01	1.970	1.280E+03
220	75-69-4	TRICHLOROFLUOROMETHANE	O	4.013E+00	2.130	1.100E+03
221	1582-09-8	TRIFLURALIN	O	2.012E-03	4.137	6.000E-01

CD	FINAL_CAS	FINAL_CONTAMINANT	TYPE	H	LOG KOC	SOLUBILITY
224	108-05-4	VINYL ACETATE	O	2.114E-02	0.342	3.025E+04
225	75-01-4	VINYL CHLORIDE	O	1.150E+00	1.040	8.800E+03
226	95-47-6	XYLENES (TOTAL)	O	2.140E-01	2.110	2.424E+02

APPENDIX 4 – PARTITION COEFFITIONS AND DEGRADATION RATES FOR METALS AND INORGANIC COMPOUNDS

The following table presents the partitioning coefficients for inorganic and metal constituents. A more detailed description of the sources of information and the selection methods is presented in section 3.5.2.3.

Field description

- CD – Identifier number of the contaminant.
- CAS– the final CAS number used in the dilution attenuation component.
- CONTAMINANT - The final contaminant name used in the dilution attenuation component.
- The log(Kd) value selected. The minimum Log(Kd) was selected from the available references.
- Degradation Rate- The degradation rate used in the assessment.

(1) US.EPA, 1996. Attachment C. Chemical properties

(2) U.S EPA, 2000. Attachment C - Radiological properties for SSL development, Soil Screening Guidance for Radionuclides

(3) Schwarzenbach et al, 1993. Environmental organic chemistry.

CD	CAS	Contaminant	TYPE	H	Final LOG(KD)	(1) Log(Kd) From Chemical properties PH=6.8	(2) Log(Kd) from Radiological document	Degradation Rate 1/day	COMMENTS
227	15176-26-8	Zinc ion	M	0.00E+00	-1.00	1.79	-1.00	4.710E-06	
223	none	none	M	0.00E+00	-0.40	None	-3.979E-01	7.327E-16	
222	15086-10-9	TRITIUM	I	0.00E+00	-18.00	None	-1.800E+01	2.747E-07	
212	7440-14-4	Radium Isotop	M	0.00E+00	0.48	None	4.77E-01	2.061E-09	
210	7440-28-0	THALLIUM	M	0.00E+00	-18.00	1.85	-18.00	8.242E-07	
203	14808-79-8	SULFATE	I	0.00E+00	0.70	None	None	0.000E+00	Kd same as Se
201	10098-97-2	STRONTIUM-90	M	0.00E+00	0.00	None	0.00E+00	1.137E-07	
200	14701-18-9	Strontium ion	M	0.00E+00	0.00	None	0.00E+00	2.383E-05	
198	17341-25-2	Sodium ion	M	0.00E+00	-18.00	None	-1.80E+01	0.000E+00	
196	14701-21-4	Silver ion	M	0.00E+00	0.43	0.92	0.43	0.000E+00	
195	7782-49-2	SELENIUM	M	0.00E+00	0.70	0.70	None	0.000E+00	
192	10043-92-2	Radon	I	4.39E+00	-18.00	None	-1.800E+01	3.008E-04	H From Schwarzenbach (3)
191	15262-20-1	RADIUM-228	I	0.00E+00	0.48	None	4.771E-01	4.121E-07	
190	13982-63-3	RADIUM-226	I	0.00E+00	0.48	None	4.771E-01	2.061E-09	
181	14797-73-0	PERCHLORATE	I	0.00E+00	-18.00	None	None	0.000E+00	
170	14797-65-0	NITRITE	I	0.00E+00	-18.00	None	None	0.000E+00	
169	none	NITRATE+NITRITE	I	0.00E+00	-18.00	None	None	0.000E+00	
168	14797-55-8	NITRATE	I	0.00E+00	-18.00	None	None	0.000E+00	
167	14701-22-5	Nickel ion	M	0.00E+00	1.53	1.81	1.53	0.000E+00	
153	14302-87-5	Mercury ion	M	0.00E+00	1.72	1.72	None	0.000E+00	
152	14333-14-3	Manganate	M	0.00E+00	0.69	None	6.90E-01	0.000E+00	
151	14581-92-1	Magnesium ion	M	0.00E+00	0.00	None	None	0.000E+00	Kd same as Sr
147	14701-27-0	Lead ion	M	0.00E+00	0.78	None	7.78E-01	0.000E+00	
144	15438-31-0	Iron Ion	M	0.00E+00	0.49	None	4.91E-01	0.000E+00	
141	15035-72-0	Sulfide	I	4.09E-01	-18.00	None	None	0.000E+00	H from Schwarzenbach (3)
129	16984-48-8	FLUORIDE	I	0.00E+00	-18.00	None	None	0.000E+00	
97	57-12-5	CYANIDE	I	3.41E-03	-18.00	None	None	0.000E+00	H from Schwarzenbach (3
94	17493-86-6	Copper ion	M	0.00E+00	0.78	None	None	0.000E+00	Kd same as lead
90	17493-86-6	Chromate	M	0.00E+00	1.28	1.28E+00	None	0.000E+00	Kd value is for chromate which is a weaker adsorber
85	16887-00-6	CHLORIDE	I	0.00E+00	-18.00	None	None	0.000E+00	
80	3812-32-6	CARBONATE	I	1.18E+03	-18.00	None	None	0.000E+00	
75	14102-48-8	Calcium cation	M	0.00E+00	0.00	None	None	0.000E+00	Kd equal to Sr

CD	CAS	Contaminant	TYPE	H	Final LOG(KD)	(1) Log(Kd) From Chemical properties PH=6.8	(2) Log(Kd) from Radiological document	Degradation Rate 1/day	COMMENTS
74	22537-48-0	Cadmium cation	M	0.00E+00	0.43	1.88	0.43	0.000E+00	
66	24959-67-9	BROMIDE	I	0.00E+00	-18.00	None	None	0.000E+00	
64	11113-50-1	Boric acid	I	0.00E+00	-18.00	None	None	0.000E+00	
63	71-52-3	BICARBONATE	I	1.17E+00	-18.00	None	None	0.000E+00	
62	14701-08-7	Beryllium ion	M	0.00E+00	2.90	2.90	None	0.000E+00	
54	16541-35-8	Barium Cation	M	0.00E+00	1.61	1.61	None	0.000E+00	
52	1332-21-4	ASBESTOS	I	0.00E+00	-18.00	None	None	0.000E+00	
51	15584-04-0	Arsenate	M	0.00E+00	1.46	1.46	None	0.000E+00	
49	64924-52-3	Antimonate	M	0.00E+00	-18.00	None	-18.00	0.000E+00	
47	14903-36-7	Aluminum Cation	M	0.00E+00	0.49	None	None	0.000E+00	Kd same as iron

APPENDIX 5 - DEGRADATION RATES FOR ORGANIC COMPOUNDS

The following table presents the degradation rates selected for the organic constituents. A more detailed description of the sources of information and the selection methods is presented in section 3.5.2.4.

Field description

- CD – Identifier number of the contaminant.
- CAS– the final CAS number used in the dilution attenuation component.
- CONTAMINANT - The final contaminant name used in the dilution attenuation component.
- Half Life – The estimated half-life of the contaminant in hours.
- Degradation – The degradation rate computed from the half-life.

* GW = Groundwater, SW = Surface water

CD	CONTAMINANT	CAS	HALF LIFE (Hours)		Degradation rate (1/day)	
			GW	SW	GW	SW
1	1,1,1,2-TETRACHLOROETHANE	630-20-6	1604	1604	1.801E-05	1.801E-05
2	1,1,1-TRICHLOROETHANE	71-55-6	13104	6552	2.204E-06	4.408E-06
3	1,1,2,2-TETRACHLOROETHANE	79-34-5	1056	1440	2.735E-05	2.006E-05
4	1,1,2-TRICHLOROETHANE	79-00-5	17520	8760	1.648E-06	3.297E-06
5	1,1-DICHLOROETHANE	75-34-3	8640	3696	3.343E-06	7.814E-06
6	1,1-DICHLOROETHYLENE	75-35-4	3168	4320	9.117E-06	6.685E-06
7	1,1-DICHLOROPROPENE	563-58-6	450	900	6.418E-05	3.209E-05
8	1,2,3-TRICHLOROBENZENE	87-61-6	720	1440	4.011E-05	2.006E-05
9	1,2,3-TRICHLOROPROPANE	96-18-4	17280	8640	1.671E-06	3.343E-06
10	1,2,4-TRICHLOROBENZENE	120-82-1	8640	4320	3.343E-06	6.685E-06
11	1,2,4-TRIMETHYLBENZENE	95-63-6	1344	900	2.149E-05	3.209E-05
12	1,2-DICHLOROETHANE	107-06-2	8640	4320	3.343E-06	6.685E-06
13	1,2-DICHLOROPROPANE	78-87-5	61872	30936	4.668E-07	9.336E-07
14	1,2-DIPHENYLHYDRAZINE	122-66-7	8640	1740	3.343E-06	1.660E-05

CD	CONTAMINANT	CAS	HALF LIFE (Hours)		Degradation rate (1/day)	
15	1,3,5-TRIMETHYLBENZENE	108-67-8	450	900	6.418E-05	3.209E-05
16	1,3-DICHLOROBENZENE	541-73-1	8640	4300	3.343E-06	6.717E-06
17	1,3-DICHLOROPROPANE	142-28-9	450	900	6.418E-05	3.209E-05
18	1,3-DICHLOROPROPENE	542-75-6	450	900	6.418E-05	3.209E-05
19	2,2-DICHLOROPROPANE	594-83-2	450	900	6.418E-05	3.209E-05
20	2,3,7,8-TCDD	1746-01-6	28320	14160	1.020E-06	2.040E-06
21	2,4,5-T	93-76-5	4320	900	6.685E-06	3.209E-05
22	2,4,5-TP	93-72-1	450	900	6.418E-05	3.209E-05
23	2,4,6-TRICHLOROPHENOL	88-06-2	43690	1440	6.610E-07	2.006E-05
24	2,4-D	94-75-7	4320	900	6.685E-06	3.209E-05
25	2,4-DICHLOROPHENOL	120-83-2	1032	900	2.799E-05	3.209E-05
26	2,4-DINITROPHENOL	51-28-5	12624	3840	2.288E-06	7.521E-06
27	2,4-DINITROTOLUENE	121-14-2	8640	900	3.343E-06	3.209E-05
28	2,6-DINITROTOLUENE	606-20-2	8640	900	3.343E-06	3.209E-05
29	2-CHLOROTOLUENE	95-49-8	450	900	6.418E-05	3.209E-05
30	2-HEXANONE	591-78-6	104	208	2.777E-04	1.389E-04
31	2-METHYLPHENOL	95-48-7	336	360	8.596E-05	8.023E-05
32	3-HYDROXYCARBOFURAN	16655-82-6	450	900	6.418E-05	3.209E-05
33	4-CHLOROTOLUENE	106-43-4	450	900	6.418E-05	3.209E-05
34	4-ISOPROPYLTOLUENE	99-87-6	180	360	1.605E-04	8.023E-05
35	4-METHYL-2-PENTANONE	108-10-1	336	360	8.596E-05	8.023E-05
36	ACENAPHTHENE	83-32-9	4896	900	5.899E-06	3.209E-05
37	ACENAPHTHYLENE	208-96-8	2880	1440	1.003E-05	2.006E-05
38	ACETOCHLOR	34256-82-1	720	1440	4.011E-05	2.006E-05
39	ACETONE	67-64-1	336	360	8.596E-05	8.023E-05
40	ACRYLONITRILE	107-13-1	1104	552	2.616E-05	5.232E-05
41	ALACHLOR	15972-60-8	720	1440	4.011E-05	2.006E-05
42	ALDICARB	116-06-3	15240	8664	1.895E-06	3.333E-06
43	ALDICARB SULFONE	1646-88-4	450	900	6.418E-05	3.209E-05
44	ALDICARB SULFOXIDE	1646-87-3	450	900	6.418E-05	3.209E-05
45	ALDRIN	309-00-2	28400	14200	1.017E-06	2.034E-06
48	ANTHRACENE	120-12-7	22080	1440	1.308E-06	2.006E-05
50	AROCLOR	53469-21-9	1800	3600	1.605E-05	8.023E-06
53	ATRAZINE	1912-24-9	720	1440	4.011E-05	2.006E-05
55	BENTAZON	25057-89-0	450	900	6.418E-05	3.209E-05
56	BENZENE	71-43-2	17280	900	1.671E-06	3.209E-05
57	BENZO(A)ANTHRACENE	56-55-3	32640	1440	8.848E-07	2.006E-05
58	BENZO(A)PYRENE	50-32-8	720	1440	4.011E-05	2.006E-05
59	BENZO(B)FLUORANTHENE	205-99-2	29280	1440	9.864E-07	2.006E-05
60	BENZO(G,H,I)PERYLENE	191-24-2	31200	15600	9.257E-07	1.851E-06
61	BENZO(K)FLUORANTHENE	207-08-9	102720	1440	2.812E-07	2.006E-05
65	BROMACIL	314-40-9	450	900	6.418E-05	3.209E-05
67	BROMOBENZENE	108-86-1	450	900	6.418E-05	3.209E-05

CD	CONTAMINANT	CAS	HALF LIFE (Hours)		Degradation rate (1/day)	
68	BROMOCHLOROMETHANE	74-97-5	180	360	1.605E-04	8.023E-05
69	BROMODICHLOROMETHANE	75-27-4	450	900	6.418E-05	3.209E-05
70	BROMOFORM	75-25-2	8640	4320	3.343E-06	6.685E-06
71	BROMOMETHANE	74-83-9	912	672	3.167E-05	4.298E-05
72	BUTACHLOR	23184-66-9	450	900	6.418E-05	3.209E-05
73	BUTYL BENZYL PHTHALATE	85-68-7	4320	360	6.685E-06	8.023E-05
76	CARBARYL	63-25-2	1440	900	2.006E-05	3.209E-05
77	CARBOFURAN	1563-66-2	450	900	6.418E-05	3.209E-05
78	CARBON DISULFIDE	75-15-0	180	360	1.605E-04	8.023E-05
79	CARBON TETRACHLORIDE	56-23-5	8640	8640	3.343E-06	3.343E-06
81	CHLORDANE	57-74-9	66528	33264	4.341E-07	8.682E-07
82	CHLORDANE (ALPHA-CHLORDANE)	5103-71-9	1800	3600	1.605E-05	8.023E-06
83	CHLORDANE (GAMMA-CHLORDANE)	12789-03-6	1800	3600	1.605E-05	8.023E-06
84	CHLORDANE (TRANS-NONACHLOR)	39765-80-5	1800	3600	1.605E-05	8.023E-06
86	CHLOROBENZENE	108-90-7	7200	3600	4.011E-06	8.023E-06
87	CHLOROETHANE	75-00-3	1344	672	2.149E-05	4.298E-05
88	CHLOROFORM	67-66-3	43200	4320	6.685E-07	6.685E-06
89	CHLOROMETHANE	74-87-3	1344	672	2.149E-05	4.298E-05
91	CHRYSENE	218-01-9	48000	1440	6.017E-07	2.006E-05
92	CIS-1,2-DICHLOROETHYLENE	156-59-2	450	900	6.418E-05	3.209E-05
93	CIS-1,3-DICHLOROPROPENE	10061-01-5	450	900	6.418E-05	3.209E-05
96	CYANAZINE	21725-46-2	1800	3600	1.605E-05	8.023E-06
98	DALAPON	75-99-0	2880	1440	1.003E-05	2.006E-05
99	DCPA DI-ACID DEGRADATE	2136-79-0	720	1440	4.011E-05	2.006E-05
100	DCPA MONO-ACID DEGRADATE	887-54-7	720	1440	4.011E-05	2.006E-05
101	DDE	72-55-9	270000	3600	1.070E-07	8.023E-06
102	DI-(2-ETHYLHEXYL)ADIPATE	103-23-1	1344	672	2.149E-05	4.298E-05
103	DI-(2-ETHYLHEXYL)PHTHALATE	117-81-7	9336	550	3.094E-06	5.251E-05
104	DIAZINON	333-41-5	450	900	6.418E-05	3.209E-05
105	DIBENZ(A,H)ANTHRACENE	53-70-3	45120	1440	6.401E-07	2.006E-05
106	DIBROMOCHLOROMETHANE	124-48-1	4320	4320	6.685E-06	6.685E-06
107	DIBROMOCHLOROPROPANE	67708-83-2	450	900	6.418E-05	3.209E-05
108	DIBROMOMETHANE	74-95-3	1344	672	2.149E-05	4.298E-05
109	DICAMBA	1918-00-9	450	900	6.418E-05	3.209E-05
110	DICHLORODIFLUOROMETHANE	75-71-8	8640	4320	3.343E-06	6.685E-06
111	DICHLOROMETHANE	75-09-2	1344	900	2.149E-05	3.209E-05
112	DIELDRIN	60-57-1	51840	25920	5.571E-07	1.114E-06
113	DIETHYL PHTHALATE	84-66-2	2688	1344	1.074E-05	2.149E-05
114	DIMETHYL PHTHALATE	131-11-3	336	360	8.596E-05	8.023E-05
115	DI-N-BUTYL PHTHALATE	84-74-2	552	336	5.232E-05	8.596E-05
116	DINOSEB	88-85-7	5904	2952	4.892E-06	9.784E-06
117	DIQUAT	2764-72-9	180	360	1.605E-04	8.023E-05

CD	CONTAMINANT	CAS	HALF LIFE (Hours)		Degradation rate (1/day)	
118	DISULFOTON	298-04-4	1008	900	2.865E-05	3.209E-05
119	DIURON	330-54-1	450	900	6.418E-05	3.209E-05
120	ENDOTHALL	145-73-3	104	208	2.777E-04	1.389E-04
121	ENDRIN	72-20-8	1800	3600	1.605E-05	8.023E-06
122	EPTC	759-94-4	450	900	6.418E-05	3.209E-05
124	ETHYL METHACRYLATE	97-63-2	180	360	1.605E-04	8.023E-05
125	ETHYLBENZENE	100-41-4	5472	360	5.278E-06	8.023E-05
126	ETHYLENE DIBROMIDE	106-93-4	2880	4320	1.003E-05	6.685E-06
128	FLUORENE	86-73-7	2880	1440	1.003E-05	2.006E-05
130	FONOFOS	944-22-9	450	900	6.418E-05	3.209E-05
132	GLYPHOSATE	1071-83-6	180	360	1.605E-04	8.023E-05
136	HEPTACHLOR	76-44-8	1800	3600	1.605E-05	8.023E-06
137	HEPTACHLOR EPOXIDE	1024-57-3	26496	13248	1.090E-06	2.180E-06
138	HEXACHLOROBENZENE	118-74-1	100272	50136	2.880E-07	5.761E-07
139	HEXACHLOROBUTADIENE	87-68-3	8640	4320	3.343E-06	6.685E-06
140	HEXACHLOROCYCLOPENTADIENE	77-47-4	1800	3600	1.605E-05	8.023E-06
142	INDENO[1,2,3,CD]PYRENE	193--39-5	35040	6000	8.242E-07	4.814E-06
143	IODOMETHANE	74-88-4	1344	672	2.149E-05	4.298E-05
145	ISOPROPYLBENZENE	98-82-8	384	360	7.521E-05	8.023E-05
146	LAMBAST	845-52-3	720	1440	4.011E-05	2.006E-05
148	LINDANE	58-89-9	5765	5765	5.010E-06	5.010E-06
149	LINURON	330-55-2	8544	4272	3.380E-06	6.761E-06
150	P XYLENE	106-42-3	180	360	1.605E-04	8.023E-05
154	METHIOCARB	2032-65-7	450	900	6.418E-05	3.209E-05
155	METHOMYL	16752-77-5	180	360	1.605E-04	8.023E-05
156	METHOXYCHLOR	72-43-5	8760	3600	3.297E-06	8.023E-06
157	METHYL ETHYL KETONE	78-93-3	336	360	8.596E-05	8.023E-05
158	METHYL METHACRYLATE	80-62-6	1344	672	2.149E-05	4.298E-05
159	METHYL-T-BUTYL ETHER	1634-04-4	8640	4320	3.343E-06	6.685E-06
160	METOLACHLOR	51218-45-2	720	1440	4.011E-05	2.006E-05
161	METRIBUZIN	21087-64-9	450	900	6.418E-05	3.209E-05
162	MOLINATE	2212-67-1	450	900	6.418E-05	3.209E-05
164	M-XYLENE	108-38-3	8640	672	3.343E-06	4.298E-05
165	NAPHTHALENE	91-20-3	3192	900	9.048E-06	3.209E-05
166	N-BUTYLBENZENE	104-51-8	180	360	1.605E-04	8.023E-05
171	NITROBENZENE	98-95-3	9456	4728	3.054E-06	6.109E-06
172	N-PROPYLBENZENE	103-65-1	180	360	1.605E-04	8.023E-05
174	ORTHO-1,2-DICHLOROBENZENE	95-50-1	8640	4320	3.343E-06	6.685E-06
175	OXAMYL	23135-22-0	450	900	6.418E-05	3.209E-05
176	O-XYLENE	95-47-6	8640	672	3.343E-06	4.298E-05
178	PARA-1,4-DICHLOROBENZENE	106-46-7	8640	4320	3.343E-06	6.685E-06
179	PCBs	53469-21-9	1800	3600	1.605E-05	8.023E-06
180	PENTACHLOROPHENOL	87-86-5	36480	3600	7.917E-07	8.023E-06

CD	CONTAMINANT	CAS	HALF LIFE (Hours)		Degradation rate (1/day)	
183	PHENANTHRENE	85-01-8	9600	1440	3.008E-06	2.006E-05
184	PICLORAM	1918-02-1	720	1440	4.011E-05	2.006E-05
185	PROMETON	1610-18-0	720	1440	4.011E-05	2.006E-05
186	PROPACHLOR	1918-16-7	450	900	6.418E-05	3.209E-05
187	PROPAZINE	139-40-2	720	1440	4.011E-05	2.006E-05
188	P-XYLENE	106-42-3	8640	672	3.343E-06	4.298E-05
189	PYRENE	129-00-0	91200	1440	3.167E-07	2.006E-05
193	RDX	121-82-4	450	900	6.418E-05	3.209E-05
194	S-BUTYLBENZENE	135-98-8	180	360	1.605E-04	8.023E-05
197	SIMAZINE	122-34-9	720	1440	4.011E-05	2.006E-05
202	STYRENE	100-42-5	5040	672	5.730E-06	4.298E-05
204	T-BUTYLBENZENE	98-06-6	450	900	6.418E-05	3.209E-05
206	TERBACIL	5902-51-2	450	900	6.418E-05	3.209E-05
207	TERBUFOS	13071-79-9	450	900	6.418E-05	3.209E-05
208	TETRACHLOROETHYLENE	127-18-4	17280	8640	1.671E-06	3.343E-06
209	TETRAHYDROFURAN	109-99-9	180	360	1.605E-04	8.023E-05
211	TOLUENE	108-88-3	672	528	4.298E-05	5.470E-05
215	TOXAPHENE	8001-35-2	1800	3600	1.605E-05	8.023E-06
216	TRANS-1,2-DICHLOROETHYLENE	156-60-5	450	900	6.418E-05	3.209E-05
217	TRANS-1,3-DICHLOROPROPENE	10061-02-6	450	900	6.418E-05	3.209E-05
218	TRIAZINES	122-34-9	720	1440	4.011E-05	2.006E-05
219	TRICHLOROETHYLENE	79-01-6	39672	8640	7.280E-07	3.343E-06
220	TRICHLOROFLUOROMETHANE	75-69-4	17280	8640	1.671E-06	3.343E-06
221	TRIFLURALIN	1582-09-8	1800	3600	1.605E-05	8.023E-06
224	VINYL ACETATE	108-05-4	180	360	1.605E-04	8.023E-05
225	VINYL CHLORIDE	75-01-4	69000	4320	4.186E-07	6.685E-06
226	XYLENES (TOTAL)	95-47-6	8640	672	3.343E-06	4.298E-05

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